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FY06 NRL DoD High Performance Computing Modernization Program Annual Reports

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Introduction

This book is a compilation of reports on all the work accomplished by NRL scientists and engineers and their collaborators using the DoD High Performance Computing Modernization Program's (HPCMP) resources for fiscal year 2006. The reports encompass work performed by researchers at all three NRL sites: Washington, DC; Stennis Space Center, Mississippi; and Monterey, California.

These reports are categorized according to the primary Computational Technology Area (CTA) as specified by the HPCMP, and include resources at the Major Shared Resources Centers as well as the Distributed Centers. This volume includes three indexes for ease of reference. These are an author index, a site index, and an NRL hierarchical index of reports from the Branches and Divisions in the Laboratory.

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Computational Structural Mechanics

- High-resolution, multidimensional modeling of materials and structures subjected to a broad range of impulsive loading that ranges from weak to intense.

- DoD application areas include conventional underwater explosion and ship response, structural acoustics, coupled field problems, space debris, propulsion systems, structural analysis, total weapon simulation, lethality/survivability of weapon systems (e.g., aircraft, ships, submarines, tanks), theater missile defense lethality analysis, optimization techniques, and real-time, large-scale soldier and hardware-in-the-loop ground vehicle dynamic simulation.

Title: Two-Dimensional Arrays of Nanomechanical Resonators
Author(s): Jeffrey W. Baldwin, Martin Marcus, Maxim K. Zalalutdinov, and Brian H. Houston
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CSM

Computer Resources: Linux Networx Cluster [ARL, MD]

Research Objectives: The fundamental research objective is to conduct advanced modeling of nanomechanical systems which augments our current fabrication and measurement capabilities. A computational model of a nanomechanical array of coupled resonators has been made to support ongoing basic research where these systems are being studied experimentally. Specifically, we wish to quantify the 1-D and 2-D localization lengths associated with disorder.

Methodology: Specialized finite element software capable of millions of degrees of freedom and advanced matrix techniques are necessary for the computations of the large, multi-element arrays modeled in these systems. In addition, with tens of thousands of eigenvalues needed in a system with two million degrees of freedom, the most sophisticated parallel eigenvalue analysis software is needed. Modal analysis is performed based on numerical simulations that employ finite elements methods (FEM) to predict the response of these arrays. Shell-type elements were used to model the resonators as plates, free on the outside and clamped on the pillars' edges. Counting the number of the normal modes of the array per frequency interval provides us with the density of states (DOS) for our "artificial crystals". The materials (silicon, for example) are generally anisotropic lending more difficulty and complexity to the problem. These systems have very high quality factors (Q) and low loss factors, which means a very high frequency refinement must be used over a large range of frequencies (kHz – GHz) to fully capture the structural response. This response is post-processed to obtain the mechanical energy broken down into it component forms. The analysis gives accurate frequency placement of the bandpass and stopbands in arrays of 2D nanomechanical resonators, which is a first step towards realizing the possibilities of nanomechanical systems for chem-bio sensing or RF signal processing.

Results: The inset of Figure 1 demonstrates the DOS for a 10x10 array of the plate resonators shown in the SEM image. The DOS plot shows two distinct acoustic bands (45-50 MHz and 65-95 MHz) separated by a pronounced bandap. Inspection of the mode shapes of the array and cross-referencing with the modes of a single paddle resonator indicate that the low frequency band of the array's DOS is being populated by the "bridge-type" modes produced by the motion of the connecting arms, while the upper band is filled with a variety of modes stemming from the square plate itself. Experimental observation of the predicted band structure in our microfabricated resonator arrays (Figure 2), estimation of the localization range for the collective modes, and evaluation of the disorder effects were the initial research goals. Numerical prediction of the array performance is key to the design of an optimized array. The direct counting of the number of peaks in the lower band provides an estimation of 12 MHz^{-1} for the DOS. This number is almost an order of magnitude lower than the value expected from FEM analysis. We attribute this discrepancy to the fact that only a limited number of resonators surrounding the driving point is participating in the collective modes. We suggest that the propagation of the elastic waves over the array is limited by the Anderson's localization and is determined by "disorder," i.e., mistune of the resonators forming our artificial crystal. We conclude that the array has an effective size of approximately 10x10 which leads to a theoretical prediction of the DOS that is in good agreement with the experimental value.

Significance: The use of HPC computing time greatly decreases the fabrication-testing iteration time. Using the HPC computers, calculations run in minutes instead of days/weeks. There is significant cost savings to the development of nanomechanical resonator based systems. We believe this work will lead to mechanical-based high frequency (GHz) signal processing elements, ultra-fast single atomic mass unit mass detectors, and picoTesla magnetometers.

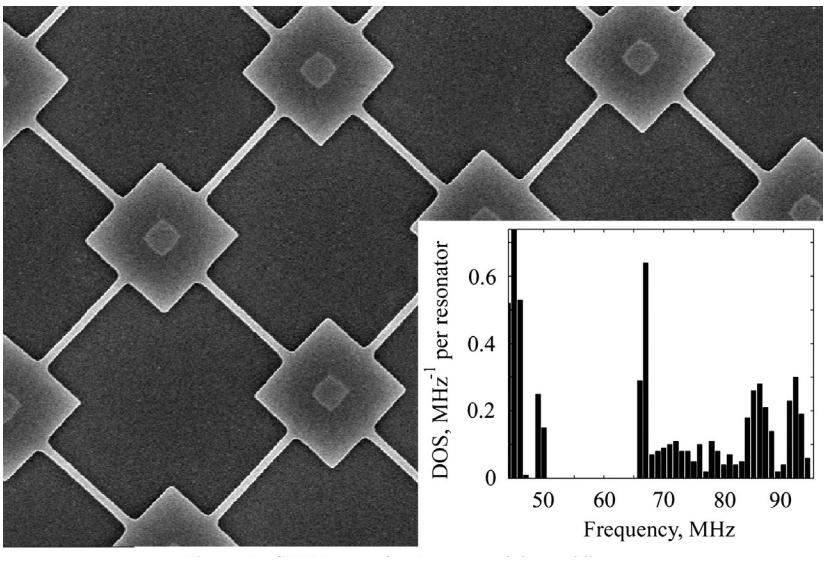


Figure 1. SEM image showing part of the paddle resonator array. The dimensions of the silicon square paddles are 2 x 2 μm, thickness 45 nm. The SiO_2 pillar supporting the center of the paddle has a cross section 0.54 x 0.54 μm and is 150 nm tall. The connecting bars are 2 μm long and 200 nm wide. Inset shows the results of finite element analysis for the density of states in the 10 x 10 paddle array. DOS was calculated by direct counting of the number of modes (deduced from FEM modal analysis) per frequency interval.

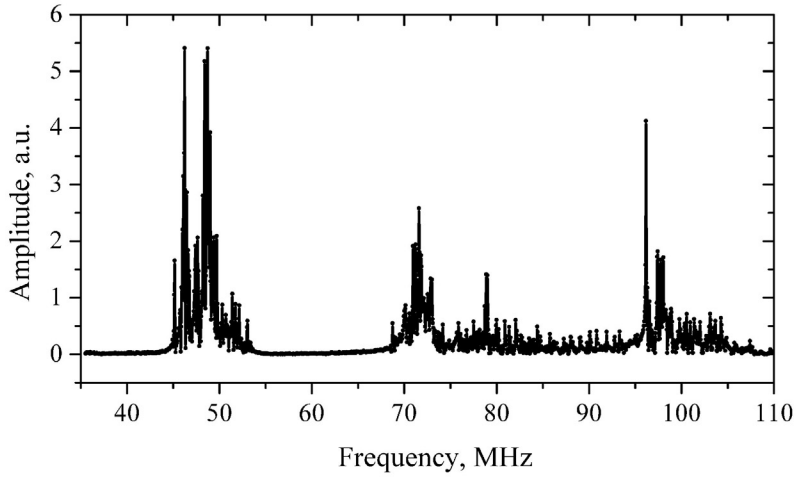


Figure 2. Frequency response of 20 x 20 paddle array with 2-μm-long connecting arm. Data acquired by driving a paddle at the center of the array and detecting the vibrations at the next paddle.

Title: Geometric, Constitutive and Loading Complexities in Structural Materials
Author(s): A. B. Geltmacher[1], S. A. Wimmer[1], V. G. DeGiorgi[1], A. C. Leung[1], J. N. Baucom[1], A. C. Lewis[1], and M. S. Qidwai[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]SAIC, Washington, DC
CTA: CSM

Computer Resources: SGI Altix and Compaq SC 45 [ASC, OH]

Research Objectives: The research objective is developing a rational basis and mathematical description of complex material response for traditional structural materials, composites and novel evolving materials. The technical approach utilizes state of the art computational methods to model complex interactions both at and across scales. Scales of consideration include microscale, mesoscale and macroscale. Parameters of interest define constitutive response (bulk and component material), kinematics nonlinearities, geometric complexities, loading path dependence, rate dependence, and interaction between loading types (i.e., electrical and mechanical). Work is not limited to structural performance of materials.

Methodology: The project uses finite element techniques extensively but the work is not limited to finite element methodologies. Other traditional, such as boundary element, and non-traditional, such as cellular automaton, techniques are explored and used as considered beneficial to the work. Nonlinear material mechanical constitutive response features are highlighted in much of work the performed. Implicit and explicit solutions methods are used as appropriate. The primary finite element code used is ABAQUS. User subroutines are used for specialized material constitutive response. Coupled material responses, such as electrical-thermal for capacitor materials or electrical-mechanical for piezoelectric materials are exercised for evaluation of these effects. ABAQUS Viewer, Tecplot, Matlab, and MSC PATRAN are used for visualization of results, including animation. ABAQUS CAE, CUBIT, MSC PATRAN and in-house software are used for model development.

Results: This project involves work in several topical areas. Work has been performed on the development of image-based microstructural models in 3D, strain and stress state visualization, material processing of multi-layer composites, prognostics modeling for material damage and fracture, and cellular automaton-based damage models. Representative results for one topic are presented here.

Design of Naval Steels: Mesoscale image-based modeling was conducted using 3D reconstructions of actual AL6XN microstructures to simulate the role of microstructure on the continuum-level response of a material. These mesoscale image-based models are finite element simulations use spatial information of microstructural features such as grain morphology, crystallographic grain orientation and boundary types. The finite element analyses were used to predict the role of the actual 3D microstructure on the generation of local stress and strain states for different loading directions and level of constraint. Typical results are shown in Figure 1 for a 0.2% applied strain in the x-direction. The present analyses were focused on the three-dimensional network of grain boundaries, and the interactions of the applied strains with different types of boundaries and junctions, as shown in Figure 2. Under uniaxial tensile loading conditions, the highest stresses were observed at $\Sigma 3/\Sigma 3$ triple junctions. When the microstructure was loaded in shear, however, this trend is not observed, and the value of von Mises stress at these junctions is in some cases lower than at other junctions.

Significance: The adaptation of new materials and the adaptation of existing materials to new uses require understanding material characteristics and the ability to accurately predict performance. In the above example, the computational models are expected to be used as a guide and evaluation tool for the development of physical prototypes.

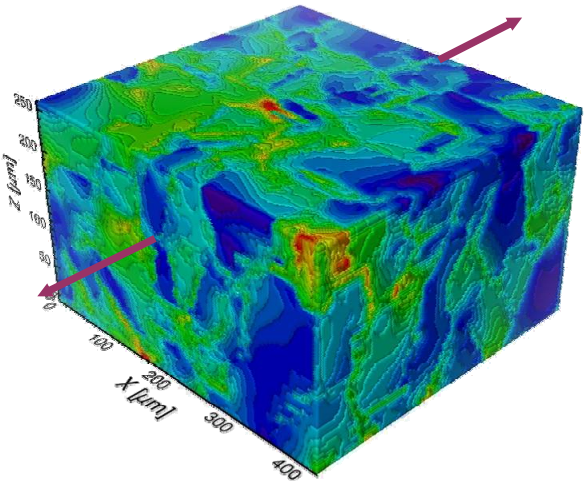


Figure 1. Contour plots of von Mises stress as a result of a 0.2% applied strain in the x-direction, as indicated in the figure.

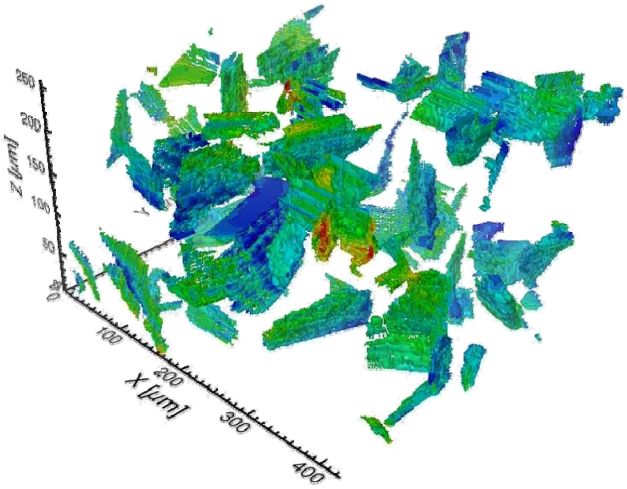


Figure 2. von Mises stress contours plotted on only the surfaces representing Σ3 boundaries in the microstruture.

Computational Fluid Dynamics

- Accurate numerical solution of the equations describing fluid and gas motion and the related use of digital computers in fluid dynamics research.
- For basic studies of fluid dynamics, for engineering design of complex flow configurations, for predicting the interaction of chemistry with fluid flow for combustion and propulsions for interpreting and analyzing experimental data, and for extrapolating into regimes that are inaccessible or too costly to study.
- Encompasses all velocity regimes and scales of interest to the DoD without restrictions on the geometry and the motion of boundaries defining the flow.
- The physics to be considered may entail additional force fields, coupling surface physics and microphysics, changes of phase, change of chemical composition, and interactions among multiple phases in heterogeneous flows.

Title: Contaminant Transport and Source Simulations for Urban and Environmental Hazard Assessment
Author(s): Theodore R. Young[1], Jay Boris[1], Keith Obenschain[1], Gopal Patnaik[1], MiYoung Lee[2], and Adam Moses[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]Berkley Research Associates, Beltsville, MD
CTA: CFD

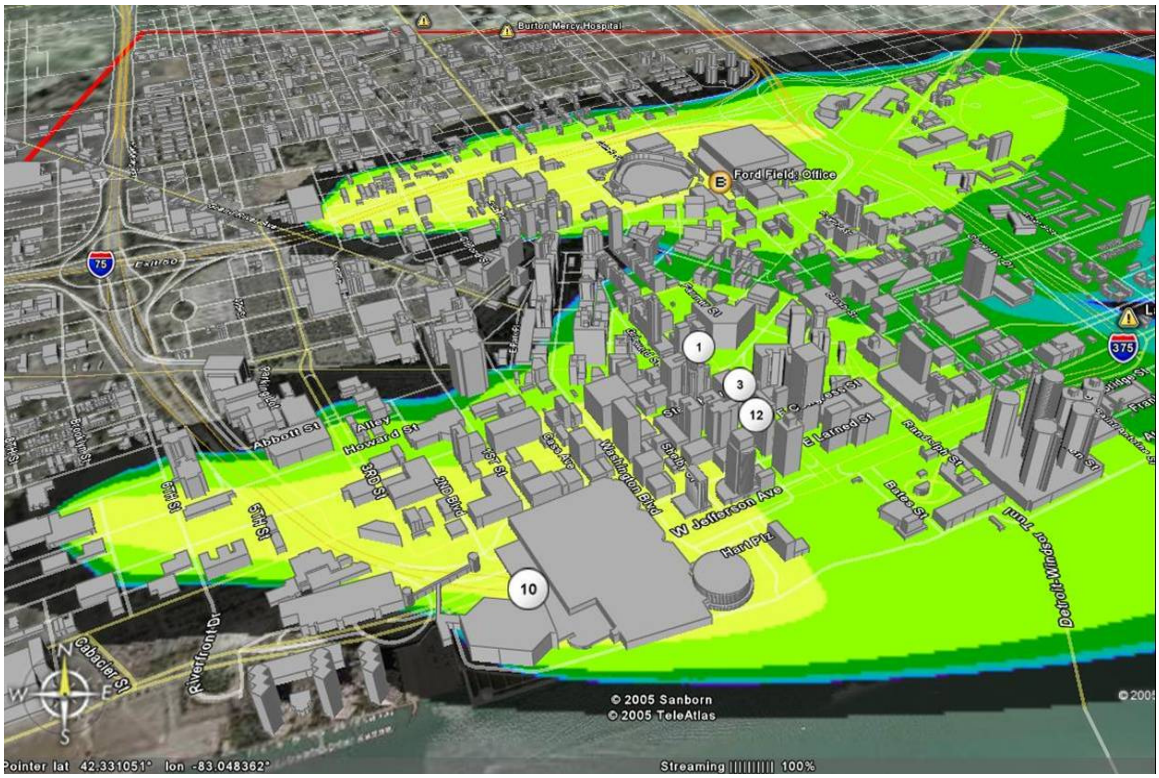
Computer Resources: IBM P4 [ARL, MD]; SGI Altix [NRL, DC]

Research Objectives: Perform high-resolution detailed 3D CFD simulations for a variety of urban areas to construct the underlying databases for fast and accurate plume predictions.

Methodology: Use the model, FAST3D-CT, perform the time-accurate, high-resolution 3D CFD, as an offline detailed urban contaminant transport scenario generator. Data from the detailed simulations is then be distilled into a very compact data set called "Dispersion Nomografs™" that can be later utilized by CT-Analyst® to render instantaneous plume predictions, sensor fusion and placement for a variety of urban and metrological parameters and conditions.

Results: Over 150 high profile domestic cities and urban areas as well as military installations both in the US and abroad have been identified that lack adequate defense against covert or accidental release of Chemical, Radiological or Biological agents. We have prioritized this list in accordance with funding provided and need and have started the on going task of performing the 3D CFD simulations needed to build the "Dispersion Nomograf" data sets. Several cities have been partially completed to the extent to provide at least minimal defense for specific high value and sensitive areas of interest.

Significance: The Dispersion Nomografs, which are made possible on reasonable time scales by HPC resources together with CT-Analyst provide a unique defensive capability for first responders, disaster response planning and post incident mop up. In addition to instantaneous very accurate plume prediction and tracking, sensor fusion and placement, CT-Analyst gives the unique capability to backtrack and determine the location of an unknown source simply based on sensor readings and metrological parameters.



The figure shows two simultaneous plumes depicted by CT-Analyst in conjunction with Google Earth made possible with the dispersion Nomograf data set built from the Detailed 3D FAST3D-CT simulations of this area.

Title: Unsteady Air-Wakes for Ship Topside Design
Author(s): W. C. Sandberg[1], F. Camelli[2], and R. Löhner[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]George Mason University, Fairfax, VA
CTA: CFD

Computer Resources: SGI-Altix, [NRL, DC]

Research Objectives: The study for topside air-wake flow and stack gas simulations for ships is a time consuming process. The current project involves the analysis of air-wake and temperature for the LPD17. The overall goal of these computations is to understand the impact of the air-wake in the landing process. Extending the air-wake knowledge to the existing procedures for landing, such as landing period designator, will lead to improvements in the landing process.

Methodology: The steps in any of these simulations are: geometry reconstruction from CAD or blue print information, tessellation of the computational domain, solution of the partial differential equations with their boundary conditions, and visualization and analysis of the solution. The solution step is one of the most time consuming in the whole process, e.g., this step took in the order of months in the LPD-17 and T-AKE-1 studies. An unstructured-grid based LES solver was used to compute the unsteady aerodynamics about the ship superstructure due to the combined affects from the ship forward speed and the incident wind including variable wind gusting.

Results: The unsteady air-wake for the LPD17 has been extensively studied. We have analyzed real time histories for 0, 15, 30, 45 and 60 degrees wind from port and from 15 degrees starboard. All these runs have been carried out at the NRL facilities, using the two ALTIX systems, niobe and morpheus. We have identified very high velocity gradient zones which could be hazardous for air vehicle operations. An example of this is shown in Figure 1.

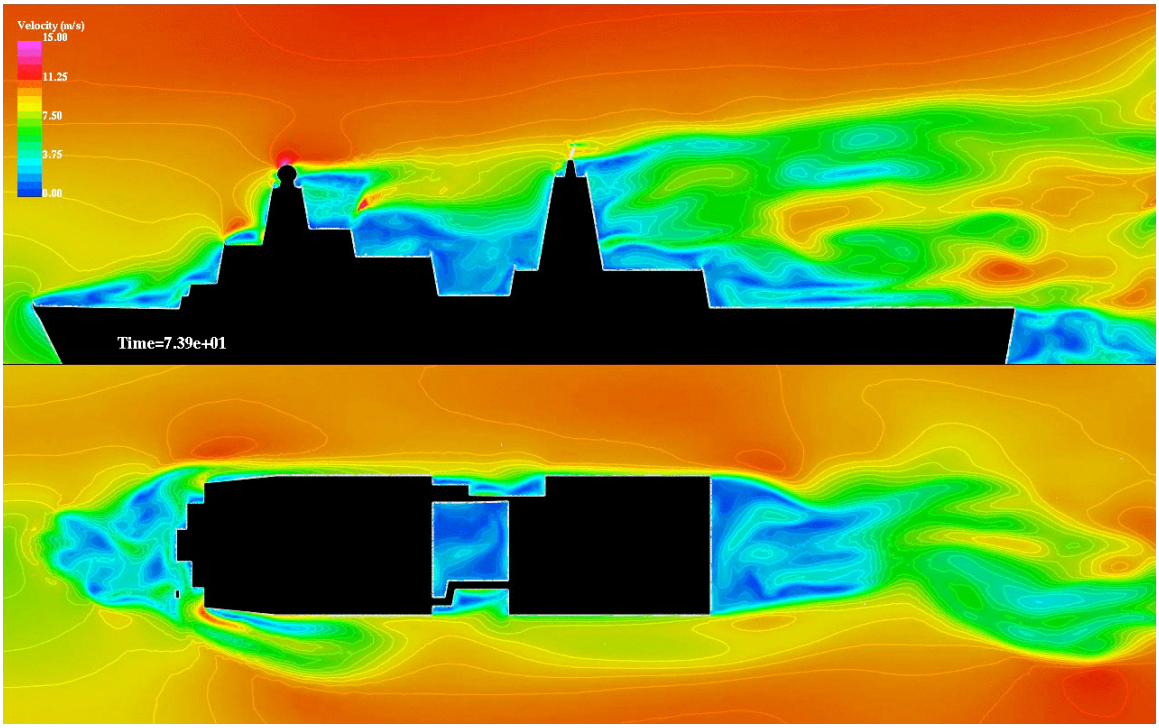


Figure 1. Vertical and horizontal planes indicating zones of high velocity gradients that may be hazardous for air vehicle operations aboard the LPD-17 Class ships.

Title: Dynamic Phenomena in the Solar Atmosphere
Author(s): Spiro K. Antiochos, C. Richard DeVore, and Mark G. Linton
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray T3E, Cray X1E [AHPCRC, MN]; SGI Origin 3900 [ASC, OH], [ERDC, MS]; SGI Altix [NRL, DC]; Linux Cluster [ASC, OH]; Cray XD1 [NRL, DC]

Research Objectives: The goal of this HPC program is to understand and to model the solar drivers of the violent space weather that disrupts DoD and civilian communications, navigation and surveillance systems. The program is focused on understanding, and ultimately predicting, the initiation process of the most important solar driver: coronal mass ejections(CME). The fundamental question that we are investigating with our numerical simulations is whether magnetic reconnection leads to the giant disruptions of the Sun's magnetic field that constitute a CME/eruptive solar flare event.

Methodology: During the past few years, we have developed a theoretical model for CME initiation: the "breakout" model. In previous numerical simulations we showed that the breakout model can produce a fast ejection in both 2.5D and 3D systems. During the past year we concentrated on two important issues: (1) Demonstrating how magnetic reconnection can produce the 3D sheared-arcade magnetic topology that leads to explosive eruption and that is required by the breakout model. (2) Understanding the role of 3D reconnection in producing the intense post-CME heating observed as an X-ray flare. For these investigations we used our ARMS code which incorporates a dynamically adaptive numerical mesh in either Cartesian or spherical coordinates. ARMS uses our state-of-art FCT technology to solve both the ideal and resistive MHD equations. We also used our 3D pseudo-spectral code CRUNCH3D for problems that allowed for periodic boundary conditions.

Results: With ARMS we simulated the interaction of pairs of distinct prominences formed by the photospheric line-tied shearing of two separated dipoles. One case was typical of solar observations of prominence merging, in which the prominences have the same axial field direction and sign of magnetic helicity. For that configuration, we found the formation of linkages between the prominences due to magnetic reconnection of their sheared fields. We analyzed the evolution of the plasma-supporting magnetic dips in this configuration and found that the dips evolve so that they increasingly fill the volume between the prominences, and the two progenitors gradually merge into a single prominence. Our model reproduces typical observational properties reported from both high-cadence and daily observations at various wavelengths. The resulting magnetic topology differs significantly from that of a twisted flux tube and is fully compatible with the sheared arcade model for the pre-eruption field. In addition to the pre-eruption topology, we investigated the post-eruption magnetic evolution. We showed, theoretically and via MHD simulations, how a short burst of localized reconnection on a current sheet creates a pair of reconnected flux tubes. We found that slow-mode shocks propagate along these reconnected flux tubes, releasing magnetic energy as in steady state Petschek reconnection. The geometry of these three-dimensional shocks, however, differs significantly from the classical two-dimensional geometry. Based on our results, we argued that the descending coronal voids seen by Yohkoh SXT, LASCO, and TRACE are reconnected flux tubes descending from a flare site in the high corona, for example after a coronal mass ejection. In this model, these flux tubes would then settle into equilibrium in the low corona, forming an arcade of postflare coronal loops as observed.

Significance: The numerical results and comparison with observation provide strong support for our breakout model for the origin of coronal mass ejections. Furthermore, our simulations yield important new information on the amount and form of the energy that is released by these explosive events. These results have greatly advanced our understanding and ability to forecast the primary drivers of space disturbances.

Title: Simulations of the Ionosphere and Magnetosphere
Author(s): S. P. Slinker[1], J. D. Huba[1], M. Swisdak[1], P. Schuck[1], and G. Joyce[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]ICARUS, Washington, DC
CTA: CFD

Computer Resources: SGI Origin [ASC, OH], [ERDC, MS]; SGI Altix [NRL, DC], [ASC, OH]

Research Objectives: Develop space weather forecasting capability. Simulate geomagnetic storms and other events of interest in order to understand the Earth's magnetosphere and ionosphere and to improve the model.

Methodology: The simulation model is a three-dimensional magnetohydrodynamics model of the Earth's magnetosphere. Measured solar wind data are used as input conditions to drive the system. Currents in the inner boundary are closed in the ionosphere where an elliptic potential equation is solved. The Origin and Altix versions of the model use OpenMP.

Results: Magnetic and electric fields from the simulation were used by our collaborators to push solar wind and outflowing polar cap ions. These studies illustrate the sources of the magnetospheric plasma. Populating the inner magnetosphere with oxygen ions from the ionosphere during geomagnetic disturbances was demonstrated. The simulation of the large geomagnetic storm which occurred on 20-21 November 2003 was completed: a period of over 32 hours of real time. The fields and potentials from this run will be used to study ring current development. The geomagnetic storm of 14-15 January 1988 was revisited. Runs were made where the magnetosphere simulation was driven by the solar wind conditions derived from the NRL CME flux rope model of Chen and Krall. The results were used as input to the NRL SAMI3 ionosphere model which can predict the ionospheric total electron content (TEC). The TEC is an important parameter needed to understand propagation of electromagnetic signals.

Several smaller studies were also undertaken. Polar cap energy deposition was studied for the events of 28 March 1998. To assist the GEM investigation of the measurement of field aligned currents by the Iridium satellite constellation, we performed simulation of the events of 31 August 2001, 1 August 2000, 16 July 2000, and 11 September 2000.

Significance: Potential protection of communication satellites and the power grid. Support of ongoing experiments in remote sensing of the space environment. Provide input to ionospheric and thermospheric models.

Title: Deforming Free Surface Flows
Author(s): W. C. Sandberg[1], C. Yang[2], and R. Löhner[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]George Mason University, Fairfax, VA
CTA: CFD

Computer Resources: SGI Altix [NRL, DC]

Research Objectives: The computation of flows with free surface is difficult, especially if the interface separates fluids of dramatically different densities, such as air and water. Neither the shape nor the position of the interface between gas and liquid is known a priori; on the contrary, it often involves unsteady fragmentation and merging process. The modeling and computation of highly nonlinear unsteady free-surface flows are currently an area of strong activity in the computational community. The research objective of the current project is to extend an unstructured-grid-based incompressible Euler/Navier-Stokes solver to handle the highly nonlinear free surface flows via the VOF techniques. In addition we are seeking to compute the forces on vehicles very near the interface, both above it and below it.

Methodology: As the objective of this study is to model the highly nonlinear free surface flows, one of the most promising interface-capturing methods -- VOF method is adopted and further developed. In the present study, an unstructured grid based solver for the incompressible Navier-Stokes equations has been extended to handle the highly nonlinear free surface flows via the VOF techniques. A fixed grid is used which covers the space occupied by both the liquid and the gas phase. Since the grid does not follow the deformation of the free surface, the grid movement is only necessary if the shape or location of the solid boundary changes.

Results: Computations have been carried out for a vehicle traveling both above and below the free surface. Shown in Figure 1 is the free surface pressure distribution for the vehicle translating just beneath the free surface which can be examined to determine the energy transferred from the vehicle into the formation of waves (wave resistance). In addition all other components of drag have been computed in order to determine the total power requirements of the vehicle.

Significance: A robust Volume of Fluid (VOF) technique has been developed and coupled with an incompressible Euler/Navier Stokes solver operating on adaptive, unstructured grids to simulate the operation of a vehicle beneath the free surface. This capability will enable examination of various vehicle operating modes.

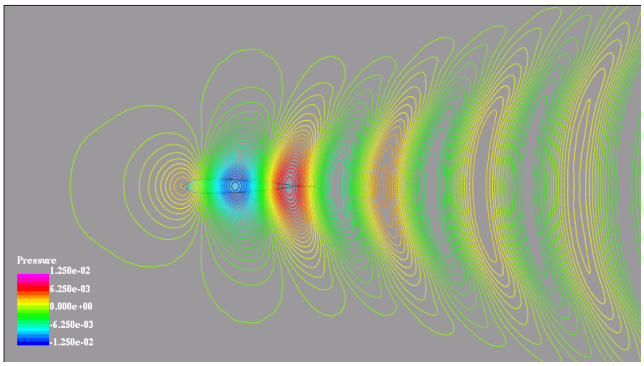


Figure 1.

Title: Adaptive Re-meshing for Unsteady Flight in Insects and Fishes
Author(s): W. C. Sandberg[1], R. Ramamurti[1], and R. Löhner[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]George Mason University, Fairfax, VA
CTA: CFD

Computer Resources: SGI Altix [NRL, DC]

Research Objectives: Develop adaptive re-meshing strategies and computational technology for unsteady incompressible flows past flapping and deforming surfaces. Utilize these methods to investigate the mechanisms of lift and thrust production in very large amplitude non-linear wing and fin motions in insects and fish.

Methodology: An implicit finite element solver, FEFLOIC, for 3-D incompressible flows based on unstructured grids was used as the primary flow solver. This model is one of the DoD HPC benchmark codes. The flow solver was combined with adaptive re-meshing techniques for these transient problems with moving grids and was also integrated with the rigid body motion in a self-consistent manner which allowed the simulation of fully coupled fluid-rigid body interaction problem of arbitrary geometric complexity in three dimensions. New re-meshing routines were incorporated into this code.

Results: 3-D unsteady CFD simulations were successfully carried out to model the dynamics behavior of insect flight and fish swimming. A deformable fin design was evaluated throughout the stroke cycle to determine if sufficient thrust was produced. Assessment of flapping air vehicle designs were also carried out.

Significance: Flapping control surfaces which are capable of generating high lift or thrust at low speeds are of immense value to the Navy. Underwater research vessels operate at low speeds where conventional control surfaces are quite poor. Improved position control and thrust control is extremely important for carrying out missions, particularly when operating in close proximity to the bottom. Unmanned air vehicles may benefit from flapping modes of propulsion as vehicle size and operating speed are decreased. A computational capability to design low speed, high thrust devices and low speed high lift vehicles is quite important in developing innovative autonomous air and underwater vehicles.

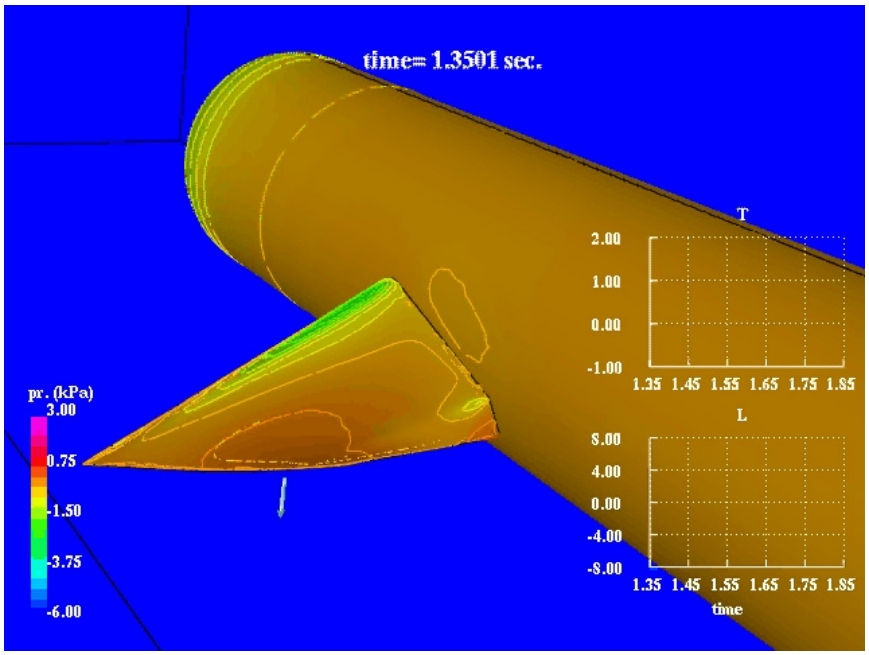


Figure 1. Thrust and lift time histories from flapping and deforming propulsor.

Title: 3D Simulations of Thermonuclear Supernovae
Author(s): Vadim N. Gamezo and Elaine S. Oran
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XD1, SGI Altix [NRL, DC]; SGI Altix, SGI Origin 3900 [ASC, OH]

Research Objectives: Model and understand three-dimensional (3D) phenomena involved in Type Ia supernova (SN Ia) explosions, including propagation of turbulent thermonuclear flames, formation of detonation waves, and propagation of the detonation through the partially burned expanding star.

Methodology: We focus at the deflagration-to-detonation transition (DDT), which is a critical unsolved problem in Type Ia supernova models. The physics of this phenomenon in Type Ia supernovae and terrestrial chemical systems is similar, but still not well understood. This similarity allow us to study DDT and validate our models using terrestrial systems. We consider a stoichiometric hydrogen-air mixture contained in a channel with obstacles, and model the flame acceleration and DDT in this channel. The numerical model is based on reactive Navier-Stokes equations coupled with the ideal-gas equation of state and a one-step Arrhenuis kinetics of energy release. The equations are solved using the explicit, second-order, Godunov-type numerical scheme incorporating a Riemann solver, and a structured adaptive mesh based on the fully threaded tree data structure.

Results: We successfully model the flame acceleration and DDT in channels with obstacles, reproduce main experimental results, and analyze underlying physical mechanisms. Basic mechanisms for the flame and flow acceleration involve thermal expansion of combustion products, shock-flame and flame-vortex interactions, and Rayleigh-Taylor, Richtmyer-Meshkov, and Kelvin-Helmholtz instabilities. The flame accelerates faster when the distance between obstacles decreases because more obstacles per unit length create more perturbations that, in turn, increase the flame surface area more quickly. The accelerating flow generates strong shocks that reflect from channel walls and obstacles and eventually create hot spots that produce detonations through Zeldovich's gradient mechanism. Shocks produce hot spots more efficiently when the obstacle spacing is large enough for Mach stems to form. The combination of these effects is responsible for three distinct regimes of flame acceleration and DDT observed in simulations. The same basic processes are responsible for DDT phenomena in more complex geometries, such as a 2D array of obstacles.

Significance: Type Ia supernovae play an important, fundamental role in astronomy, cosmology, and particle physics. Due to their extreme brightness, these supernovae are used as “standard candles” to measure distances, curvature, and the rate of expansion of the universe. Observations of distant SN Ia indicate that there exists an unknown “repulsive force” (dark energy) which acts against “normal” gravity and leads to an accelerating expansion of the universe. This poses fundamental challenges and also provides important clues to theories of matter. Understanding the physics of SN Ia explosions, and DDT phenomena in particular, is a crucial ingredient in calibrating SN Ia as distance indicators and in separating the effects of stellar evolution and supernova environment from global cosmological effects.

DDT phenomena also play an important role in terrestrial combustion. This study is relevant for a number of practical applications, including hydrogen safety and pulse-detonation engines (PDE). For example, the results summarizing the effect of obstacle spacing on flame acceleration and DDT can be directly used to design detonation initiation devices for PDE.

Title: Fine Scale Structure of the Air-Sea Interface
Author(s): Robert Handler and Geoffrey Smith
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: SGI Altix [NRL, DC]; SGI Altix [ERDC, MS]

Research Objectives: The research objective of this multi-year effort is to understand the small-scale processes at the air-sea interface, to improve understanding of remote sensing signatures, and to improve flux modeling through the coupled air-ocean interface.

Methodology: The work presented here represents the numerical component of a balanced numerical-experimental research effort aimed at improved understanding of interfacial processes. We use a pseudo-spectral code which solves the full 3D Navier-Stokes equations. The present version of the code includes buoyancy and surfactant effects. In addition, we use a compact finite difference code which allows for the simulation of two dimensional deforming interfaces, a specific example being the simulation of a spilling breaker.

Results: In FY06 we completed the following: (1) Simulations of the air-water interface were completed at $Re = 180$ and 100 statistically independent realizations of the flow were saved; (2) The complete turbulent kinetic energy and dissipation balances of the turbulence were computed; (3) Calculations of the interface were begun at $Re = 220$; (4) Preliminary 3D visualizations of the $Re = 220$ case were made and comparisons were initiated with physical experiments. In our simulations, the domain is approximately 1 meter long, 0.5 meters in width, and about 7 centimeters in depth. When we compare these results closely with those from an experiment that was performed at the University of Miami in their air-sea interaction laboratory, the agreement was quite good with respect to several parameters of interest: (1) The general cellular nature of the surface was similar in both cases; (2) The surface drift velocities were well predicted;(3) The streak spacing was well predicted. In addition, our DNS results revealed subsurface features such as the coherent vorticity field, which cannot easily be ascertained experimentally. These very encouraging results point the way to the next step which is to perform in FY07, comprehensive simulations at $Re = 270$ and $Re = 150$ so that datasets over a full range of shear stresses will be available for detailed analysis.

Significance: The primary Naval application of this work is associated with the development of inverse remote sensing algorithms and the prediction of air-sea interfacial heat, mass, and momentum fluxes. The models developed,along with the simulations, will be used to develop new techniques for interfacialflux measurements. One specific application would be to develop criteria than can be used to determine when and if subsurface wakes can be detected using thermal IR imagery.

Title: Direct Numerical Simulation of Fluid-Sediment Wave Bottom Boundary Layer
Author(s): Joseph Calantoni
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CFD

Computer Resources: Cray X1 and Cray XT3 [ERDC, MS]

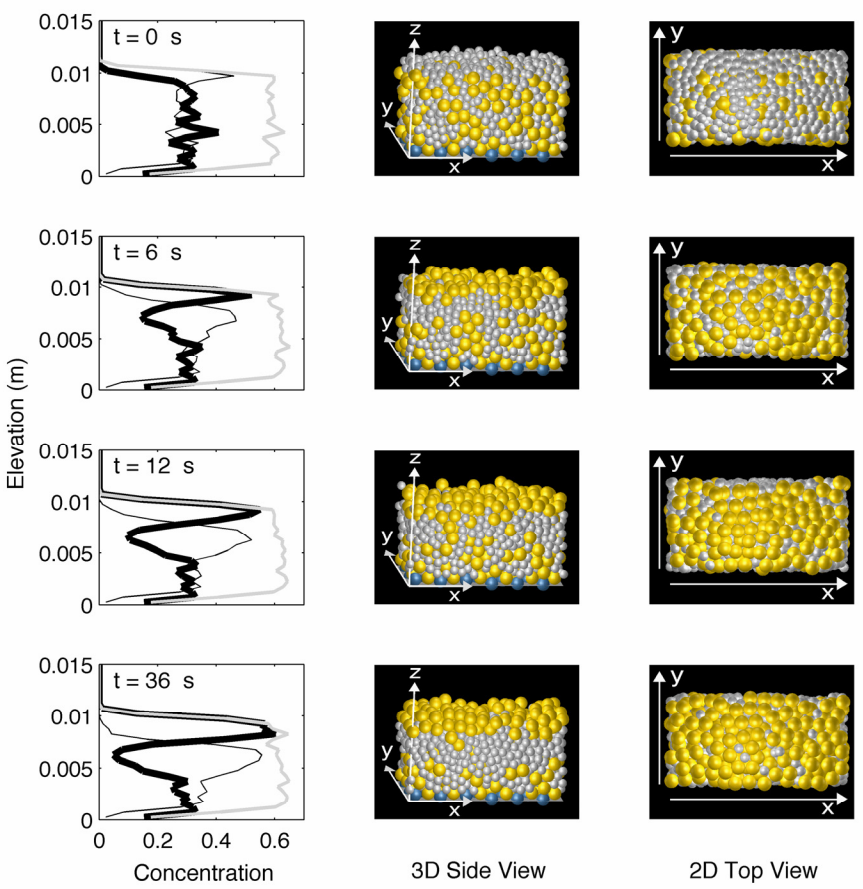
Research Objectives: The desire to develop predictive models for nearshore bathymetric evolution necessitates a better understanding of the physics of fluid-sediment interactions in the wave bottom boundary layer (WBBL). Our long-term objective is to develop robust formulae for predicting bulk sediment transport rates in the nearshore. Since such processes are difficult if not impossible to measure in-situ, we will perform numerical simulations of the two-phase (fluid and sediment) WBBL to improve existing parameterizations for bedload and suspended load transport rates in the nearshore. Fundamental concepts used in describing the phenomena of sediment transport such as the reference concentration, bed failure criterion, and more recently introduced concept of acceleration-induced transport can be addressed with our models. The models produce the high level of detail necessary to refine our present understanding of sediment transport processes and clarify new directions in the measuring techniques needed to improve present predictive capabilities.

Methodology: Utilization and development of a suite of two-phase WBBL models for simulating sediment transport in the nearshore environment is ongoing with the use of HPC resources. The three-dimensional sediment phase of the flow is simulated with a discrete element model (DEM) that allows individual grains to be uniquely specified (e.g., size, density, and shape). The fluid phase of the models varies in complexity from a simple one-dimensional eddy viscosity to a fully three-dimensional direct numerical simulation. Coupling between fluid and sediment phases varies from one-way coupling, where fluid flow drives particle motions without any feedback, to a system fully coupled at every fluid time step, where Newton's Third Law is strictly enforced.

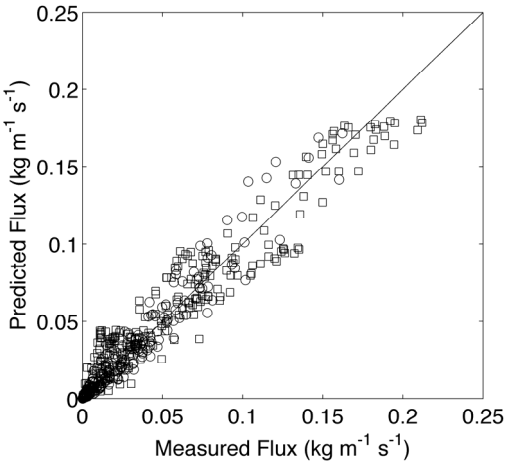
The paradigm we follow is to use a deterministic model to simulate many different cases, which in turn, allows us to develop a probabilistic description of the phenomena of interest. In this instance, we used a one-dimensional fluid model fully coupled to a three-dimensional DEM to simulate 243 unique cases of sheet flow or near sheet flow transport with bimodal distributions of coarse sediments under forcing from idealized waves typical of the surf zone. In the end, we provide a simple power law that fits all the simulation data with strong correlation.

Results: The discrete particle model was used to simulate coarse sand-sized spherical non-cohesive grains with diameters ranging from 0.00075 m up to 0.0015 m. In that range, the bimodal distributions spanned three different ratios of diameters and 9 different bed compositions, where the bed composition is the ratio of large to small grain particle mass. In total, 27 unique initial conditions were simulated each using a suite of 9 different idealized monochromatic waves. Initially mixed beds of grains undergo rapid vertical sorting (within 1-2 wave periods) and once the beds have partially sorted the results present a simple power law to parameterize the sediment transport rate (or flux) of the large and small grains from the bimodal distribution. The practical application of the power law is for use in larger scale models of nearshore morphodynamics.

Significance: Ultimately, all process-based models for nearshore bathymetric evolution are limited by shortcomings in fundamental knowledge of sediment transport. Model simulations provide an unprecedented level of detail for the study of sediment transport that is impossible to obtain with available measuring technologies in the field or laboratory. The computational resources consumed were in direct support of NRL base program "Coastal Dynamics of Heterogeneous Sedimentary Environments".



In the figure above, initially mixed beds of sediment sort such that the large grains migrate to the top of the active layer and the small grains move to the bottom of the active layer in the simulations. The left column plots the vertical concentration profiles of total (gray), large (thick), and small (thin) particles, initially (t = 0 s), after 1 wave period (t = 6 s), after 2 wave periods (t = 12 s), and after 6 wave periods (t = 36 s). Most of the vertical sorting occurs within 1-2 wave periods and can be observed visually with the corresponding 3-D simulation view in the middle column and the 2-D view of the top of the bed shown in the right column. The large particles are colored yellow and the small particles gray. The flow is along the *x*-direction, and the vertical is in the *z*-direction.



Plotted in the figure to the left is flux predicted using the new power law versus flux measured in simulations. The squares represent time-average flux of large grains, circles represent time-average flux of small grains (486 total points), and the line represents one-to-one correspondence. The power law is given as

$$\frac{Q_L}{Q_S} = K\left(\frac{M_L}{M_S}\right)^{\frac{D_L}{D_S}},$$

where Q_L and Q_S, M_L and M_S, and D_L and D_S, represent flux, mass, and diameter, of large and small grains, respectively. The strongly correlated power law is useful for predicting partial transport rates of bimodal distributions of coarse sediments in sheet flow.

Title: Suppression of Gas-Jet Fires in Large Enclosures
Author(s): Douglas A. Schwer and K. Kailasanath
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Linux Networx Cluster [ARL, MD]; SGI Altix [NRL, DC]

Research Objectives: Water-mist suppression of fires has been studied extensively both computationally and experimentally with small-scale laboratory setups, and to a lesser extent, simulations have also been done for larger scale enclosures. Although the laboratory setup has been useful in understanding the basic mechanisms of fire mitigation with water-mist, the application of these results to situations occurring on Navy vessels is not straight-forward. The current research is an attempt to address these difficulties. The main research goal of the present HPC project is to study fire suppression in both low and normal gravity environments such that suppression techniques (including both water mist and CO2) can be exploited to their full potential in both environments. The short term goal is to work closely with experimentalists at the Colorado School of Mines to validate the current fire mitigation simulation code using detailed experimental data for small-scale fires in large enclosures.

Methodology: The multi-phase simulation technique uses an Eulerian-Eulerian approach called the sectional approach, where the dispersed-phase is divided into "sections" dependent on droplet size, and each section has its own set of conservation equations. At the core of the gas-phase numerical procedure is the barely-implicit-correction flux-corrected-transport (BIC-FCT) algorithm, which has been developed for low Mach number fluid dynamics. This algorithm has been used extensively for flame and fire simulations, and has been shown to be an accurate, robust, and efficient algorithm. The dispersed-phase solution uses a simple explicit-FCT algorithm for each section, with source terms representing mass, momentum, and energy transfer between the sections and between each section and the gas-phase. An adaptive mesh refinement procedure is implemented using the PARAMESH library available from NASA Goddard Space Flight Center. In addition to handling adaptive mesh refinement, the PARAMESH library also handles parallelization of the domain using MPI and domain decomposition techniques.

Results: Both simulations and experiments conducted at the Colorado School of Mines have studied the behavior of small flames in large spaces, representing idealized incipient fire scenarios. Results have compared three-dimensional unsteady simulation results with experimental flames produced at the Colorado School of Mines, with reasonable accuracy demonstrated between the simulation and experimental results.

Significance: By understanding better how suppression works, more efficient techniques are possible that would suppress small fires much more quickly than currently available. This is especially important for long-term missions were replacement parts are not easily available or may be very expensive.

Title: Blast Mitigation in Large Enclosed Areas
Author(s): Douglas A. Schwer and K. Kailasanath
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Linux Networx Cluster [ARL, MD]; Cray XD1, SGI Altix [NRL, DC]

Research Objectives: Minimizing the damage caused by accidental and intentional explosions within enclosed spaces is an important area of research for the Navy and larger DOD communities. Damage to structures within the enclosed area is caused by both the shock wave generated by the explosive detonation, and from the quasi-static pressure rise that occurs over a much longer time-scale. Efficient computational methods are essential to effectively study this problem because of the need to resolve the first several shock reflections, and the comparatively long time periods over which the quasi-static pressure builds up. The current research focuses on generic spaces; however, our longer term objective is to be able to evaluate the effectiveness of water mist for specific spaces on ships. The main research goal of the present HPC project is to study the use of water-mist to mitigate pressure development within an enclosed space subjected to an explosive blast. The short term goal is to validate our current blast mitigation models with experiments accomplished in FY05 at NSWC.

Methodology: An Eulerian-Eulerian multi-dimensional computational model was used for the multi-phase flow-field calculations based on the Flux-Corrected Transport algorithm of Boris. The dispersed-phase is computed using the sectional approach, where droplets are grouped together into sections based on their size, and then Eulerian conservation equations are solved for each group of droplets with appropriate source terms for mass, momentum and heat transfer. Secondary reactions of explosive products mixed with air are also modeled, and play a significant role in the long-term pressure rise in enclosed areas. Two versions of the code are used, both using the same core physical models and numerical schemes. The first version uses the PARAMESH library that implements an adaptive mesh refinement procedure and parallelization using the MPI libraries and domain decomposition. Adaptive mesh refinement is excellent at efficiently capturing the shock dynamics and large gradients after the detonation of the explosive. The second version has a single mesh and uses the PARTI library for parallelization, again utilizing the MPI libraries and domain decomposition. This version is more efficient for the highly turbulent, well mixed flows that develop after several shock reflections.

Results: Experiments done recently at NSWC helped to validate the solution procedure that is used for long-term pressure rise in an enclosed area subjected to a blast. The simulations were able to explain many of the artifacts seen in the experiments, although a straight one-to-one comparison was not made. We began to address how critical water-mist parameters such as droplet size and spray distribution will effect the mitigation.

Significance: By addressing the effect of water-mist droplet size and spray distribution on blast mitigation in enclosed areas, we can help determine the feasibility of using water-mist systems for blast mitigation.

Title: Aerosol Release Experiment
Author(s): Carolyn R. Kaplan
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

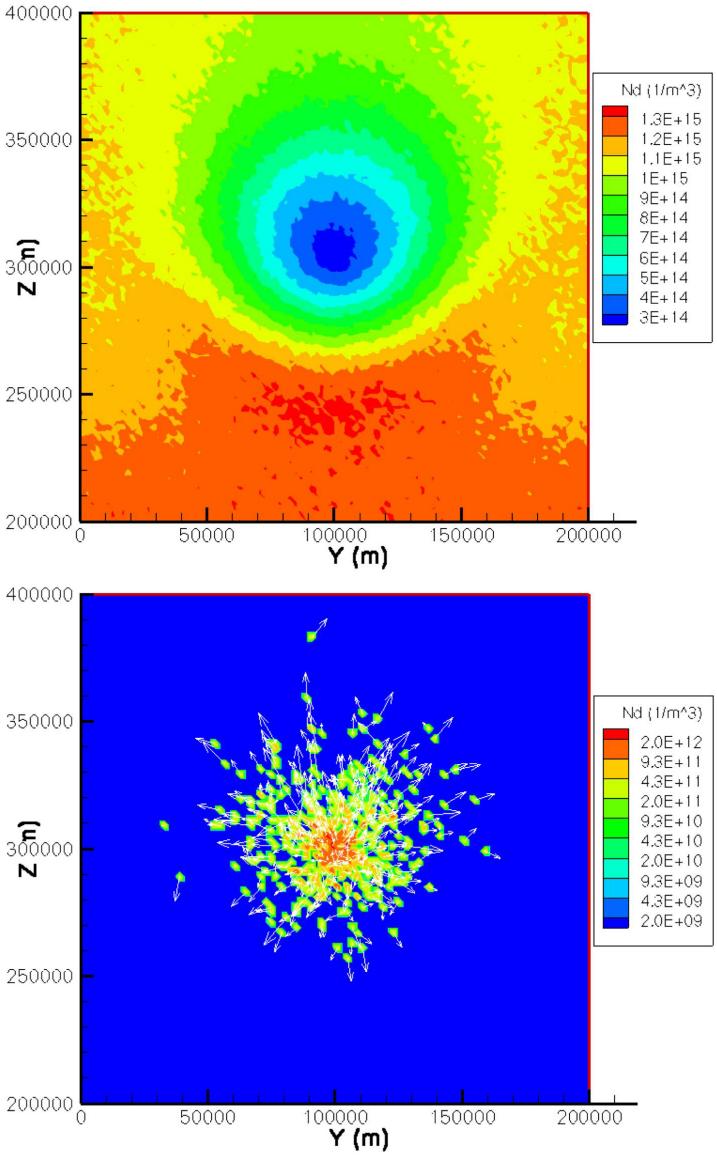
Computer Resources: SGI Altix [NRL, DC]

Research Objectives: Simulations are conducted to further study the measurements of ionospheric disturbances observed during the NRL Shuttle Ionospheric Modification with Pulsed Localized Exhaust experiments (Bernhardt et al., *J. Geophys. Res.*, 110, A05311, doi:10.1029/2004JA010795). The experiments use space shuttle orbital maneuver subsystem engines to inject high-speed exhaust molecules into the ionosphere over ground radar sites, which provide measurements of the resulting ion velocity distributions and plasma turbulence. The simulations are used to reproduce and elucidate the observed ionospheric disturbances.

Methodology: Simulations are conducted using a multi-species, reactive-flow, direct simulation Monte Carlo (DSMC) method. DSMC is regarded as a numerical solution to the Boltzmann equations; it is a statistical method, in which individual molecules are tracked through physical space, and their interactions with other molecules and with surfaces are calculated. The basic algorithm includes the following steps: move molecules, sort/index molecules, allow collisions, and then sample molecules to calculate macroscopic properties. The method assumes that molecular motion is decoupled from molecular collision during each timestep, and that the collision process (where energy is redistributed among kinetic and internal modes) is probabalistic. The DSMC methodology is well-suited for parallelization via domain decomposition. Each processor conducts its own individual DSMC calculation, and communication between processors is only necessary when a molecule crosses processor boundaries. The 3-D code is parallelized, using MPI, and was developed under the HPCMO CHSSI program. It achieves close to ideal fixed-problem speed-up on 64 processors on the Altix.

Results: The shuttle exhaust is composed of water molecules at 120K, injected into the quiescent ionosphere (at 300 km altitude) at a rate of 50×10^{25} molecules/s. The ionosphere initially consists of O^+ ions and electrons at 1000K, where the background atmospheric density decreases with altitude. The model includes two reactions: charge exchange between the shuttle exhaust and ambient atmosphere, $H_2O + O^+ \Rightarrow H_2O^+ + O$, and the ion-electron recombination reaction, $H_2O^+ + e^- \Rightarrow OH + H$. As observed experimentally by ground radar measurements, the simulations show that the injection of neutral, high-speed shuttle exhaust molecules into the background ionosphere results in the formation of an ion-ring velocity distribution and corresponding reduction in density of ambient O^+ ions (see figure). The altitude-dependent ionospheric density creates a small vertical temperature gradient in the background atmosphere, which affects the resulting flowfield. In addition, the effects of the charge exchange and ion-electron reaction (the resulting redistribution of kinetic and internal energy modes) and the injection of a high-velocity stream into a quiescent background all contribute to the formation of the observed ion-ring distribution.

Significance: Ion-ring distributions are naturally-occurring phenomena in space. These calculations (and the experiments they support) focus on the artificial generation of ion-ring velocity distributions, and are intended to simulate the naturally-occurring phenomena. Insight into the mechanisms of their formation and destruction is important to better understand the physics of space plasmas.



Distribution of ambient O^+ (top) and pick-up H_2O^+ ions (bottom) at a distance of 100 km from the shuttle exhaust. Velocity field is shown by the white vectors. Simulation results show the depletion of O^+ in the ionosphere and the ion-ring velocity distribution.

Title: Applications of FEFLO Incompressible Flow Solver
Author(s): R. Ramamurti
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

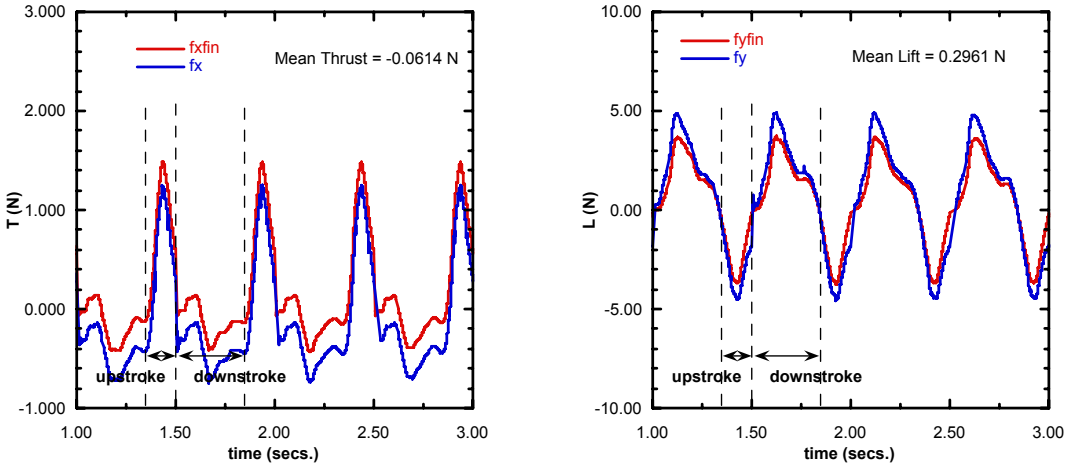
Computer Resources: SGI Altix [NRL, DC]

Research Objective: Perform three-dimensional (3-D) numerical simulations of flow past complex configurations. The proposed studies will investigate the mechanism for the thrust and lift generation and enhancement flapping wings/fins in insects and fishes and apply it UUVs.

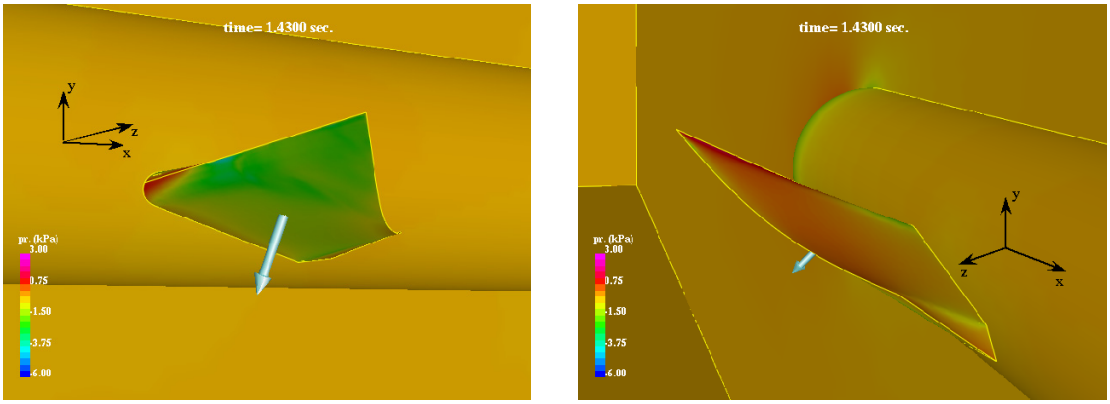
Methodology: An implicit finite element solver, called FEFLOIC, for 3-D incompressible flows based on unstructured grids is used. The flow solver is combined with adaptive remeshing techniques for transient problems with moving grids and is also integrated with the rigid body motion in a self-consistent manner which allows the simulation of fully coupled fluid-rigid body interaction problems of arbitrary geometric complexity in three dimensions. The motion of the wing/fin is prescribed from experimental observations.

Results: An application of flapping foils propulsion that was studied extensively last year is for a notional UUV with the deforming fin. For this computation, the kinematics of the Bird-wrasse pectoral fin were used on an appropriately resized fin fitted to a notional UUV. The forward velocity of the UUV was varied from 0kt to 3kts. Based on our previous study of the effect of deformation of the fin on thrust production, we have reduced the number of ribs for the mechanical fin from 14 spines in the fish to 5 ribs. This is done in order to reduce the complexity of the mechanical system. The size and the kinematics of these ribs were obtained from the pressure distribution and from the structural analysis performed in collaboration with GWU. The important parameters that govern the thrust production are the angle of attack of the root section of the fin, the frequency and the amplitude of flapping. After several parametric studies varying the angle of attack of the root section of the fin, the speed of the UUV and the flapping frequency of the fin. An angle of attack of 20° and the amplitude of the oscillation of 114° were found to be near optimum. It was found that the flapping fin was able to generate sufficient thrust to propel the UUV at 3kts with the fin flapping at 2Hz or at a speed of 1kt with the fin flapping at 1Hz.

Significance: Simulations have enabled characterization of the thrust and lift generation mechanisms in flapping foil propulsion for unmanned underwater vehicles. The flapping foil propulsion has many applications, such as submersible propulsion, maneuvering and flow control and aerodynamics of unconventional MAVs.

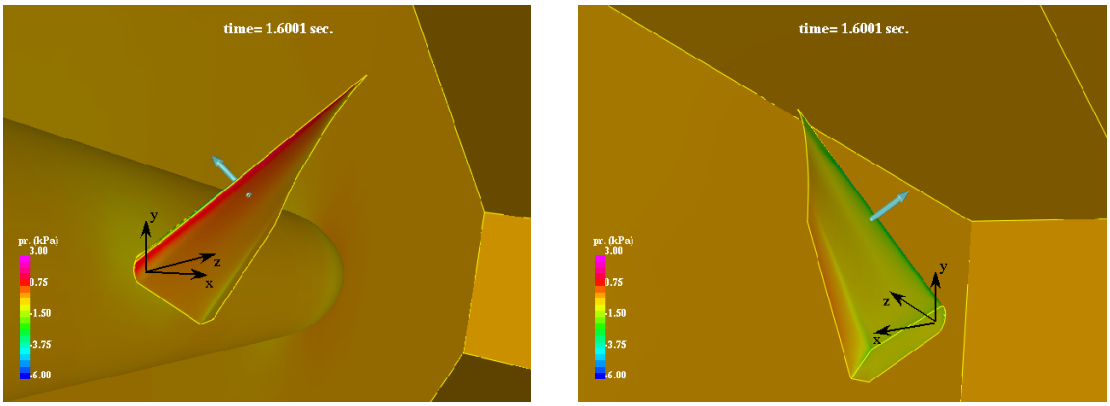


Thrust and Lift production for a UUV moving at 3 kts, $\alpha_r = 20°$, $\phi_{max} = 114°$, $f = 2.0$ Hz.



a. front view during upstroke

b. top view during upstroke



c. front view during downstroke

d. top view during downstroke

Pressure distribution on the fin at maximum thrust production instants.

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CCM

Computational Biology, Chemistry, and Materials Science

- Quantum chemistry and molecular dynamics methods are used to design new chemical systems for fuels, lubricants, explosives, rocket propellants, catalysts, and chemical defense agents.
- Solid state modeling techniques are employed in the development of high performance materials for electronics, optical computing, advanced sensors, aircraft engines and structures, semiconductor lasers, laser protection systems, advanced rocket engine components, and biomedical applications.
- These computational research tools are also used to predict basic properties of new chemical species and materials that may be difficult or impossible to obtain experimentally, such as molecular geometries and energies, spectroscopic constants, intermolecular forces, reaction potential energy surfaces, and mechanical properties.

Title: Materials for Energy Storage
Author(s): Michelle Johannes
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Altix [ASC, OH]

Research Objectives: The objective of this project is to determine the battery properties of potential electrode (cathode and anode) materials using computational methods. The eventual determination of a superior cathode material *prior* to synthesis is the ultimate goal.

Methodology: First principles pseudopotential methods will be employed to calculation the quantities of interest. The majority of the work will be done using the Vienna Ab-Initio Software Program (VASP).

Results: This project began only in August, so there have only been 2 months of work. Thus, very little can be stated in terms of results. But, preliminary testing of the methodology and comparison of the calculated quantities to experimental results were extremely positive.

Significance: The accomplished testing is significant because it provides a basis for further calculations and ensures that the project is indeed viable. The overall significance of this is far-ranging, as enormous amounts of time and money normally spent in guess-and-check synthesis of battery materials can be saved by first computing the relevant materials properties.

Title: Calculation of Materials Properties via Density Functional Theory and its Extensions
Author(s): Michael J. Mehl and Dimitrios A. Papaconstantopoulos
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Origin 3900 [ASC, OH]

Research Objectives: The determination of materials properties from accurate first-principles density functional theory (DFT) computations is limited by the small systems sizes, on the order of one hundred atoms, which can be fit onto modern computers. Even order of magnitude improvements in computational speed will only double the number of atoms in the system. Calculations of properties such as diffusion, the structure and motion of defects and dislocations, crack propagation and the electronic response of large-scale systems requires system sizes of up to one million atoms. The Center for Computational Materials Science has developed a variety of algorithms grounded in DFT and extended to handle all of these types of calculations. This project will use the techniques to study the properties mentioned above as well as other properties of materials of interest to the Navy.

Methodology: DFT computer codes will be used to expand our database of structural and electronic data high symmetry structures of systems under consideration, e.g., Fe/Cr/Ni/C for steels. This database is used used to develop parameter sets for tight-binding and atomistic potentials using codes previously developed at NRL and to augment previously developed sets of parameters. The tight-binding method, which has accuracy comparable to DFT, will be used to study systems containing thousands of atoms where the quantum mechanical nature of bonding is important. Larger systems will be studied using atomistic potentials. Unexpected predictions of these models will be verified by DFT calculations if possible.

Results: Self-interstitial atoms are produced in metals by radiation impact. This damage thus caused expands and weakens the containment vessel of a nuclear reactor, decreasing the lifetime of the reactor and requiring constant monitoring of the reactor vessel to provide early warning of a possible breach. The expansion of the reactor vessel is caused by the motion of self-interstitials through the material. This behavior has been modeled with atomistic potentials, but is difficult to do with accurate quantum mechanical studies because of computational limitations. Using the NRL Tight-Binding method we were able to successfully model the motion of self-interstitials in a variety of metals. Future work will study the interaction of these interstitials with surfaces, grain boundaries, dislocations, and point defects.

Significance: Understanding the behavior of interstitial atoms and their interaction with defects in the structure is the first step in determining ways to alleviate radiation damage in nuclear containment vessels.

Title: Growth and Control of Metal Films on Semiconductor Substrates
Author(s): S. C. Erwin
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Altix, Compaq ES40/45 [ASC, OH]

Research Objectives: To improve theoretical understanding of the surface morphology of oxides; to understand spin-polarized electron transport in organic molecules.

Methodology: This computational research is based on the generalized-gradient approximation (GGA) to density-functional theory (DFT). Semiconductor oxide surfaces and organic molecules exhibit strong distortions from ideal structures. For this reason, the most appropriate approach for the problems studied here is the pseudopotential planewave method, as implemented in the VASP code.

Results: For oxide surfaces, we showed theoretically that the triangular islands/pits reported for both ZnO(0001)-Zn and -O surfaces are not driven by electrostatics, but rather emerge from a competition between two opposing tendencies: satisfying the electron-counting rule (which favors reconstructed semiconducting surfaces) and maintaining a stoichiometric surface (which favors a unreconstructed metallic surface). For transport in molecules, our focus was on how low-energy deformations of the molecule affect the current-voltage characteristics and the magnetotransport of this molecular-scale device. We find that fairly modest deformations, costing only a few tens of meVs, can substantially change the tunneling current---by factors of two or more. Such deformations have still larger impact on the magnetoresistance, with small changes in molecular conformation even leading to changes in the sign of the magnetoresistance.

Significance: Identifying the mechanisms responsible for the morphology of surfaces is crucial to gaining better control of materials grown by epitaxial and colloidal methods, for which surface structure can strongly affect crystal quality and even impurity incorporation. The field of molecular electronics offers one possible solution to the problems faced by silicon technology as device miniaturization continues into the nanoscale regime. Some of the most interesting recent research in this field addresses the creation and detection of spin-polarized electron transport through a variety of molecular-scale conductors, including single and multiwalled carbon nanotubes, semiconductor quantum dots connected by a molecular bridge, organic thin films, and self-assembled organic monolayers. Organic molecules and films are especially promising building blocks for spin-polarized molecular electronic devices because the spin-coherence length can be much larger than in metals and traditional semiconductors.

Title: Maintaining MBD-5 CHSSI Codes for DFT Calculations Using Symmetry and Variational Fitting
Author(s): B. I. Dunlap
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Origin [NRL, DC]; IBM SP4 [ARL, MD]; Compaq SC45 [ERDC, MS]

Research Objectives: Develop fast and accurate density-functional calculations using variational fitting to reduce the formal rate at which the calculations scale to the cube of the number of occupied orbitals and to use completely analytic matrix elements to allow arbitrary accuracy.

Methodology: The codes solve the DFT equations using Gaussian basis sets to fit both the orbitals and the Kohn-Sham potential. The fits are robust, i.e., they do not change the energy to first order in the fitting error, and *all* linear-combination-of-atomic-coefficients are determined by variation. Brett Dunlap's Solid-Harmonic-Gaussian DFT (SHGDFT) uses point-group symmetry most efficiently, computes forces efficiently using the solid-harmonic basis and generalized gaunt coefficients. John Mintmire's Helical Nanostructures (HENS) can efficiently compute the electronic structure of all carbon nanotubes by explicitly treating only the rotationally equivalent atoms of the first unit cell and the helical operation.

Results: Sped up SHGDFT for low-symmetry cases such as PETN-PETN collisions by not transforming the N^3 analytic integrals needed to fit exchange when they are computed, instead transforming the set of N^2 intermediate results every SCF cycle.

Significance: The total time of PETN-PETN collision simulations was reduced by a factor of 4 on the SC45 and SP4 and a factor of 2 on the Origin computers, while keeping 75% efficiency on 64 processors vs. 32 processors.

Title: Non-equilibrium Molecular Dynamics
Author(s): Guan M. Wang and William C. Sandberg
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI-Altix [NRL, DC]

Research Objectives: The goal of the proposed research is to gain insight into the collisional dynamics of a large number of atoms in a liquid with external forces and a dilute distribution of large biomolecular fragments.

Methodology: Nonequilibrium molecular dynamics methods have been developed and used to explore a number of current research issues on fluid transport of a host liquid with large impurities present. We have used the SLLOD formulation of nonequilibrium MD with isokinetic thermostatting. We have explored both the Green-Kubo and the mean-square displacement approaches to transport computation. The VACF's have been computed in the nanochannel in a slabwise approach to determine the effects of DNA proximity. The local and long-ranged structural reorganization that occurs in the presence of external fields has also been determined.

Results: The collisional dynamics of the host liquid atoms of the system have been studied when subjected to external fields such as a velocity gradient. The velocity gradient was successfully created using moving atomic slabs. The dynamics of an ionic water solvent alone in equilibrium, an ionic water solvent being sheared, and an ionic water solvent being sheared with both free and surface-tethered DNA molecules were investigated. Appropriate boundary conditions were written and incorporated into CHARMM for the biomolecular shearing computations. The computational arrangement prior to shearing is shown in Figure 1.

Significance: These computations have successfully demonstrated the dynamics of biomolecules in a nanochannel shear flow. The techniques enable a new class of biomolecular computational analyses in non-equilibrium environments.

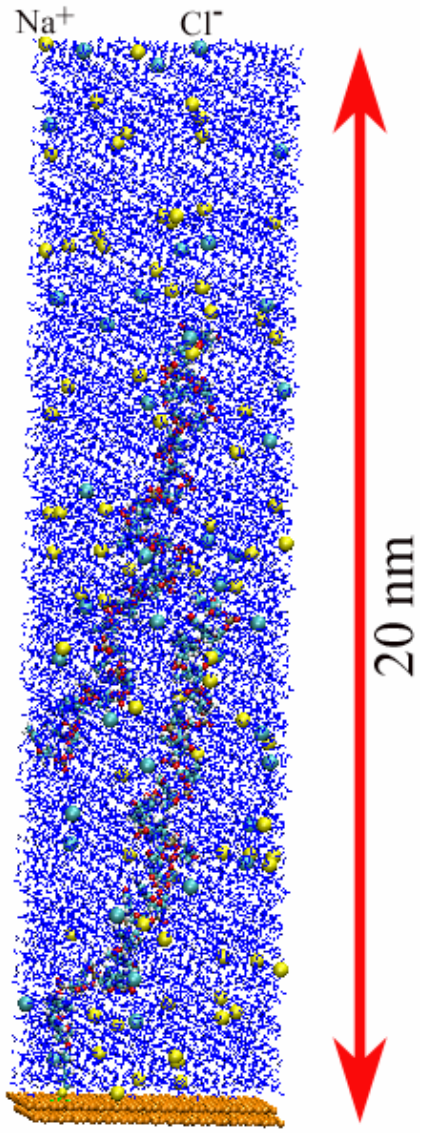


Figure 1. A double strand DNA molecule tethered to an atomic gold substrate in an ionic water solvent.

Title: Modeling Fuel Cell Chemical Reactions
Author(s): R. C. Mowrey
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Origin [ASC, OH]

Research Objectives: This project uses quantum mechanical time-dependent wave-packet methods to assess the influence of impact point, collision energy, and initial rovibrational state on the dissociation of H_2 on Pt(111). These results are relevant to developing a better understanding of the chemical reactions occurring in fuel cells.

Methodology: A four-dimensional fixed-site model is used which includes vibration, rotation, and center-of-mass translation normal to the surface. The wave function describing the motion of the nuclei is represented using a two-dimensional grid and spherical harmonic functions. An initial wave packet describing an ensemble of initial states is evolved in time by expanding the time-evolution operator in a series of complex Chebyshev polynomials. The polynomials contain damping functions to absorb the wave packet in the asymptotic regions thus preventing it from reflecting from the boundaries of the grid. The propagating wave packet is analyzed at a dividing surface outside the interaction region using the scattering amplitude formalism to compute the state-selected S-matrix and scattering probabilities. The potential energy surface describing the reaction is a fit to the results of density functional theory (DFT) calculations using a generalized gradient approximation of at Pt slab with a periodic H_2 overlayer.

Results: Figure 1 shows the dissociation probability as a function of collision energy for H_2 in the ground rovibrational state impacting at the high-symmetry top, bridge, and fcc sites. The dissociation probability becomes non-zero at low collision energies first for the top site, followed by the bridge and fcc sites, in agreement with the ordering of the potential barriers. The probability becomes non-zero at energies slightly below the potential barrier height because of tunneling and increases via a series of plateaus, eventually saturating near unity. The dynamical barrier heights (collision energy at which the reaction probability is half the saturation value) are 0.062, 0.27, and 0.37 eV, respectively. These values are in good agreement with the DFT potential barrier heights of 0.057, 0.27, and 0.42 eV. The shifts in the dynamical barrier heights relative to the potential barriers are due to the change in the zero-point energy as H_2 moves along the reaction path from the gas-phase to the potential barrier. The zero-point energy change can either increase (top site) or decrease (fcc site) the translational energy needed for dissociation. Rotational excitation (scattering of molecules back into the gas phase in a rotational state different from the incident molecule) competes with dissociation. The locations of the dips and plateaus in the dissociation curves coincide with the energies at which dissociation channels for other initial rotational states (e.g., $j=2,m_j=\pm2$) become energetically accessible. In effect, H_2 is excited to a higher rotational state at the barrier but is still able to dissociate if sufficient energy remains available to cross the potential barrier.

Significance: The calculations are in support of an ONR-supported project, "Modeling and Simulation Tools for Chemical and Electrochemical Systems: Bridging between Atomistic Fundamentals and System Engineering." The results of these calculations will used to assist in development of a new software tool to provide significant new modeling capabilities in the analysis, design, and optimization of electrochemical systems.

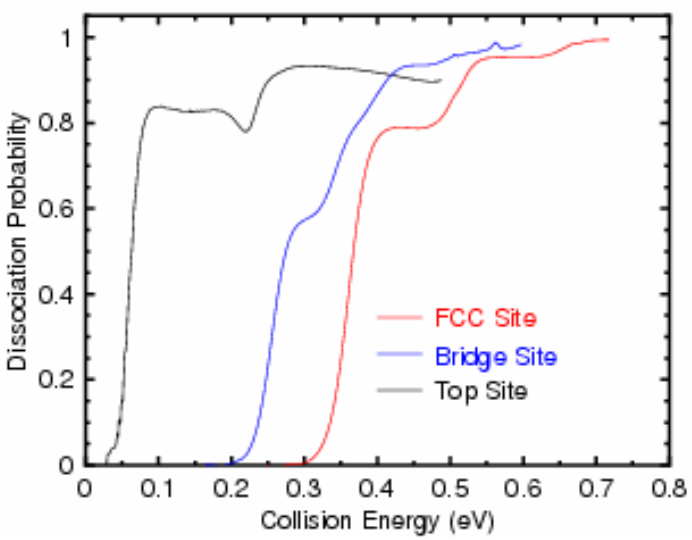


Figure 1. Dependence of reactivity on collision energy and impact site.

Title: Structural Chemistry
Author(s): Jerome Karle and Lulu Huang
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: IBM P3/P4 [MHPCC, HI]

Research Objectives: Develop and use the Kernel Energy Method to calculate larger molecules of biological interest.

Methodology: We have developed a Kernel Energy Method (KEM), for applying quantum crystallography to large molecules, with an emphasis on the calculation of the molecular energy of protein, DNA and RNA. The computational difficulty of representing the system increases only modestly with the number of atoms. The calculations are carried out on modern parallel supercomputers. By adopting the approximation that a full biological molecule can be represented by smaller "kernels" of atoms, the molecular energy is decomposed into a sum over the separate contributions of double-kernels reduced by the energy of single kernels, which otherwise would be over counted. Moreover, collections of kernels are, from a computational point of view, well suited for parallel computation.

Results: The result is a modest increase in computational time as the number of atoms increases, while retaining the *ab-initio* character of the calculations. We describe a test of our method, and establish its accuracy using protein, DNA and RNA.

Significance: The KEM in the context of quantum crystallography has been so thoroughly tested it is possible to visualize future quantum mechanical studies of applications in a host of areas, such as rational drug design, active sites of proteins, site directed mutagenesis, agricultural biotechnology, and enzyme catalysis.

Title: Modeling of Fine Water Mist/Flame Interactions
Author(s): R. C. Mowrey and R. Ananth
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Origin, SGI Altix [ASC, OH]

Research Objectives: Water mist is being developed as an alternate fire extinguishment agent for halon 1301. For water drops extinction occurs through evaporative cooling of hot gases and oxygen depletion. The interaction between water drops and fire dynamics is complex and drop size and momentum are key factors in determining the minimum amount of water needed for extinction. This project focuses on computational simulations of flame extinction in a cylindrical cup burner by water. These CFD calculations provide details on the drop dynamics, evaporation rates, chemical species concentrations, and dynamics of extinction that are not readily obtained from experimental observations.

Methodology: The commercial CFD package FLUENT was used to model the water-mist/flame interaction for a co-flow burner with a propane flame. Mono-disperse water drops were entrained in the co-flow air and transported to the flame region. A two-dimensional, axi-symmetric transient computational model was used. The drops are tracked using a Lagrangian method from the injection point until they evaporate in the flame. The reduced-chemical mechanism describing the combustion contained 35 species and 217 reactions. The size of the mesh describing the physical domain and the number of differential equations to be solved required the use of the parallel version of FLUENT. The size and mass concentration of water drops were varied to determine the conditions leading to flame extinction.

Results: The calculations show that large drops are more effective than small drops in extinguishing the flame. The water mass loading required for flame extinction increased from 10.5% to 15% as the drop size decreased from 32 μm to 4 μm. The predicted extinction concentrations are in good agreement with recent experiments performed at NRL using ultra-fine mist. Large drops penetrate the reaction kernel of the flame tip but small drops evaporate completely by the time they reach the 600 K isotherm located outside the reaction kernel. Drops that reach the attachment region surrounding the flame base reduce the rate of a critical chain branching reaction that produces OH radicals by a factor of five through evaporative cooling. The flame tip lifts up from the burner rim and blows off when the drop extinction concentration is reached. Drops that are injected close to the burner wall are carried to the flame tip and are responsible for extinction. Drops injected further from the wall evaporate downstream from the flame tip and have a negligible role in extinction.

Significance: The safety of naval vessels can be enhanced through the installation of water-mist fire suppression systems. Design of an optimal configuration for these systems is best accomplished by a combination of experimental measurements and computational modeling.

Title: Liquid Microchannel Flows for Biofluidics Analysis
Author(s): Guan M. Wang and William C. Sandberg
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

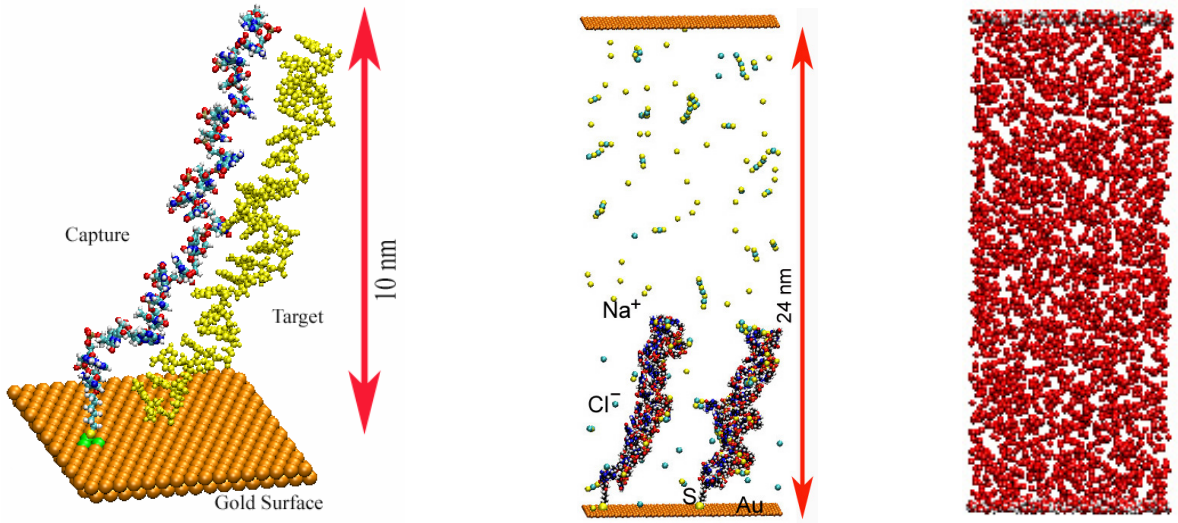
Computer Resources: SGI Altix [NRL-DC]

Research Objectives: This computational research is aimed specifically at understanding and optimizing biomolecular transport, capture, and force discrimination in microfluidic/nanofluidic systems for biological warfare (BW) threat agent detection. The development of nanosensors requires understanding of the atomic interaction dynamics of the confining nanosensor geometry, the coupling of biomolecules to the device surfaces, the molecular dynamics of the carrier solvent, and the interaction of the sensor dynamics with the carrier solvent. As for simulations of biomolecules such as DNA, at the atomic level, the study of biomolecular properties has been confined to nearly equilibrium states only, i.e., no flow fields were applied to the solvents. There has not been a way, until now, of creating shear flows in nanochannels and there has also been no capability in existence, until now, for computing the nonequilibrium dynamics of either free or tethered biomolecules.

Methodology: We have developed a series of quantum and molecular methods to enable the equilibrium software CHARMM to handle non-equilibrium dynamics. These methods have been applied to cases of DNA molecules in shear flows in nanochannels.The typical complex system that we have studied consists of DNAs tethered to Au(111) surfaces through a linker molecule 6-mercapto-1-hexanol (MCH) and a water solvent with sodium and chlorine ions. DNAs are single/double strands (ss/ds). For tethered dsDNAs only one strand is anchored onto surfaces. Free DNAs in shear flows are also explored for comparisons. The solvent contains mostly water molecules with added sodium and chloride ions to neutralize the system.

Results: We have carried out, for the first time, the all-atom computational investigation of both free and surface-tethered DNA molecules in a nanochannel shear flow. The DNA molecular relaxation time and the hydrodynamic force on DNA molecules, both free and tethered to the atomic surface wall, were directly calculated at the atomic level for the first time.

Significance: These computations will enable one to establish the flow limits for maintaining wall-attached biomolecules in nanosensor devices. The computations of the dynamics of single and multiple free ssDNA molecules in a shear flow, including the extensional and relaxational time-history, provides the first atomic-level information available to assist in understanding the behavior of long-chain polymer molecules in a shear flow and may lead to insights into the phenomena of drag reduction.



a. b. c.

Figure 1. a) One free single strand (ss) target DNA and one capture ssDNA that is tethered onto a gold surface (4.7×4.58 nm^2). These DNA single strands were drawn by separating the equilibrated configuration of an S ladder-like dsDNA. b) The MD simulation box 24 nm high with water molecules shown.

Title: Structure, Formation, and Diffusion Mechanisms in Nanostructures and Thin Films
Author(s): Michael I. Haftel and Alexander Efros
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

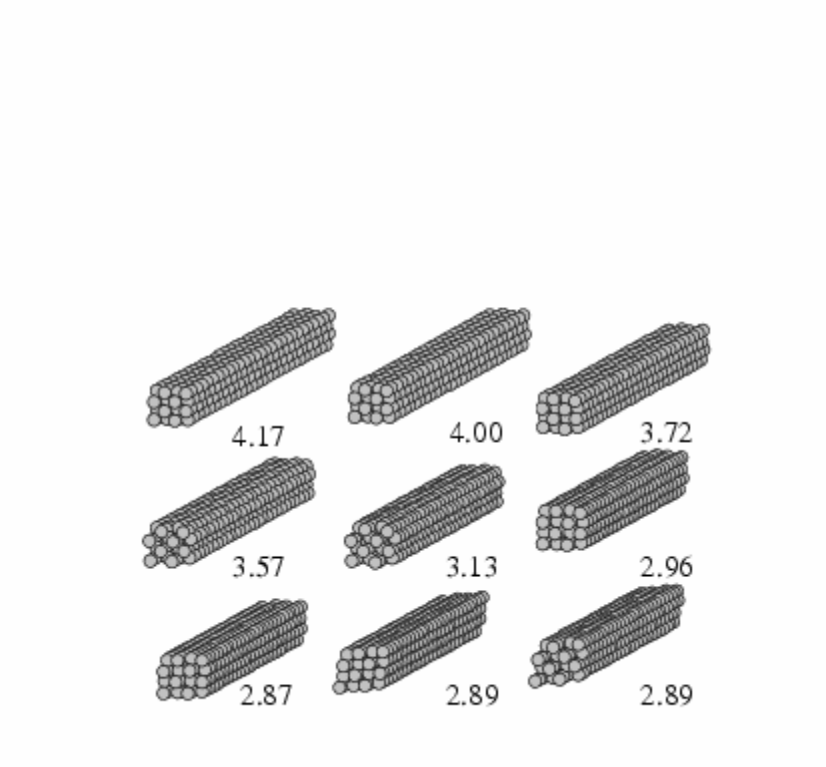
Computer Resources: Compaq SC 40/45 [ASC, OH]

Research Objectives: The main objective is to investigate the atomic structure, dynamics, and diffusion present in metal and semiconductor nanostructures, i.e., thin films, nanocrystals and nanowires. The nanostructure energetics, structure and diffusion will be analyzed, and the thermodynamics and diffusion mechanisms that account for these properties will be elucidated. From this information methods to produce nanostructures with desired features will be developed.

Methodology: The first-principles VASP code is used to calculate the structural energetics and simple diffusion processes in relatively small or symmetric systems. Moderate to large size simulations are approached through the tight-binding method or with semiempirical methods such as the surface embedded atom model (SEAM). In these cases the DAMSEL or NRL tight binding molecular dynamics (NRL-TBMD) code is utilized to simulate atomic motion or calculate structural energies.

Results: Density functional and tight binding simulations of fcc metallic nanowires were carried out with the VASP and NRL-TBMD codes to investigate structural phase transformations in these nanostructures that normally would not occur in the bulk phase. These calculations demonstrated that for diameters less than two nm, metallic fcc nanowires undergo spontaneous (under zero external stress) structural transformations that would only occur under great uniaxial stress in the bulk. Simulations were, in particular, carried out for Cu, Ni, Au, Ag and Pt. For Au and Pt suitably small fcc <001> oriented nanowires spontaneously transform to body centered tetragonal (bct) oriented in the <001> direction, whereas the other fcc <001> nanowires spontaneously reoriented to the fcc <011> direction. The critical diameters for these structural transformations were about $d<2.0$ nm, except for Au where the critical diameter was about 4.0 nm. Either type of structural transformation involves a “superelastic” response, which is the spontaneous recovery from tensile strains of 30% or more to the ground state structure of these metallic nanowires.

Significance: The nanowire simulation shows how the crystal structure can be controlled by nanowire size. The superelastic response is closely related to the shape-memory effect and demonstrates that these nanowires can be employed to obtain this effect (e.g., in actuators) in the place of exotic shape-memory alloys such as NiTi. The structural control aspect aids in the development of electro-optical materials of interest to the Navy.



Reorientation of a FCC <001> oriented Ag nanowire (upper left) to the FCC <011> orientation (lower right). The numbers indicate the longitudinal lattice constant of the nanowire in Angstroms, which undergoes a 31% contraction in the reorientation. The reorientation involves an intermediate stage of a bct structure (2.96) which has a lateral expansion and 29% longitudinal contraction.

Title: Defects in SiC
Author(s): W. E. Carlos
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI Origin [ASC, OH]

Research Objectives: The interpretation of magnetic resonance spectra of defects in semiconductors requires detailed the analysis of the nuclear hyperfine structure. This gives the chemical identity and number of the central and surrounding atoms of a defect center, essentially providing a map of its wave function. While simple atomic orbital calculations can be performed on a PC, an accurate picture must account for atomic relaxation and spin polarization effects. Once such effects are taken into consideration there can be multiple possible solutions and energy minimization schemes are required to determine the correct atomic configuration and resulting wave functions. Knowing the wave function we are then able to calculate its interaction with the electric field due to surrounding atoms (the fine structure splitting) providing a self consistent picture of the electronic and atomic structure of the defect.

Methodology: Such calculations require *ab initio* methods involving Hartree-Fock or density-functional algorithms. Fortunately, highly sophisticated quantum chemical software packages are commercially available allowing a bench scientist to perform high-level accurate calculations. Such methods are computationally intensive, well beyond the capabilities of the even the most powerful PCs, and require parallel computing for large supercells or those involving atoms in which high angular momentum atomic shells are important.

In this work, use is made of the quantum-chemical software packages available at the Aeronautical Systems Center (ASC) located at Wright-Patterson AFB. The ASC facility has, in place and ready for use, programs for *ab initio* calculations of the electronic structure of supercells containing various defects, for energy minimization to account for lattice relaxation and for spin polarization effects necessary to quantitatively compare with experimental results. The software packages include CRYSTAL03 (with CRYSTAL06 to become available shortly) and GAUSSIAN03.

Results: During the current year (FY06) a theoretical study of the defects in SiC was initiated. Preliminary calculations were performed on simple defects such as isolated vacancies and antisites which are in general agreement with results in the literature. This lead to more complex structures such as a C-Si-C trivacancy, a newly discovered defect observed in our experiments and identified with the aid of these calculations.

Significance: SiC has become the leading wide bandgap semiconductor for application in electronics for the delivery of high currents and voltages as well as in high power microwave electronics. In many of these applications deep level traps are crucial to required device performance while in others they are a critical impediment. In both instances, it is important to understand the fundamental nature of the structural defects either to optimize their concentration or to reduce the concentration to a minimal level. The addition of this quantum-chemical modeling capability has increased both the understanding of problems of current interest and the range of problems that are accessible to our work at NRL and, as a result, allowed us to leverage internal resources (e.g., an FY07 new start) and make such programs more competitive in obtaining outside funding. (We currently have funding from ONR and expect to have AFOSR funding.)

Title: Simulation and Design of Molecular Scale Materials
Author(s): Mark R. Pederson
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Linux Networx Cluster [ARL, MD]; SGI Altix and Cray XD1 [NRL, DC]; SGI Altix and Origin [ASC, OH]; IBM P3/P4 [MHPCC, HI]

Research Objectives: The objective of this research is to perform accurate density-functional calculations on novel molecular materials and to predict the behavior of such materials.

Methodology: We use a massively parallel all-electron density-functional methodology, known as NRLMOL, to predict the properties of materials. The electronic degrees of freedom are described quantum mechanically and the nuclear degrees of freedom are described clasically or within a harmonic or anharmonic quantum mechanical method. Spin-ordering and spin-orbit interactions are included.

Results: We have calculated electronic and vibrational spectra of a high-boron content cluster-based amorphous materials. The good agreement between the calculated and measured vibrational spectra suggests that the neutron-absorbing films that have a signifcant degree of disorder in them and that the solid structure is highly reconstructed in comparison to the the icosahedral boron-based feedstock used for growth. Research on the structure-function relationships in the eumelanin polymers has been completed. Work on molecular magnets continues along several new directions. First we have used the results from computational studies to predict how the magnetic properties of an Fe-based molecular magnet would be affected by control of the ligands. Second we have calculated the vibrational spectra of a mixed-metal Mo/Ni molecular magnet and also calculated the exchange interactions for this cluster. The infrared spectra is being compared to measurements due to the Musfeldt group at UT. Third we have applied a new extension of NRLMOL to the calculation of spin-dependent tunneling across molecular magnets. Work on this problem will continue into the next year. We have computationally tested a new method for calculating long-range van der Waal attractions within the density-functional theory. A new method for the efficient calcualtion of electron-vibron interactions in molecules has been tested on carbon nanotubes and several smaller molecules.

Significance: Calculations on molecular magnets provide a computational means for design and optimization of the magnetomolecular anisotropy energy and will aid in determining the feasibility for such systems for applications to magnetic storage, magnetic sensing and spintronics.

Title: Quantum-Chemical Simulation of Surface-Science Experiments
Author(s): Victor M. Bermudez
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: COMPAQ SC40/45, SGI 3900 and Altix [ASC, OH]

Research Objectives: The objective of this program is to perform quantum-chemical calculations as an aid in interpreting surface-science experiments. One example is the analysis of ultraviolet photoemission spectroscopy (UPS) data resulting from chemisorption of organic molecules on semiconductor surfaces. Extracting structural information from such data requires molecular-orbital calculations for different models and comparison with experiment. Another example is the assignment of the vibrational modes of chemisorbed species, as observed in infrared spectroscopy. This requires that one compute the energy-minimized structure and obtain the normal-mode energies for comparison with experiment.

Methodology: The CRYSTAL98 and CRYSTAL03 software packages have been used extensively. These are designed for both Hartree-Fock (HF) and Density Functional Theory (DFT) calculations on periodic structures in one, two or three dimensions. The GAUSSIAN03 software package is used for similar calculations on isolated molecules and clusters.

Results: Work has also been completed which addresses the issue of the structure and energetics of various low-Miller-index surface planes of β-Ga_2O_3 which is important in understanding the growth of nanoribbons for sensor applications. These nanostructures are single crystals with well-defined surfaces, and the calculations have determined the structure and surface energy of several surface planes that experiments have identified as important in nanoribbon growth. The electronic structure of the most stable surface has also been determined, and the band gap is found to be free of surface states. Figure 1 shows the surface band structure for the most stable surface, the (100)-B, which is nearly ideally-terminated. The results show that gap is devoid of surface states throughout the Brillouin zone.

Work has been completed on the first phase of a DTRA-funded program on quantum-chemical modeling of the adsorption of chemical warfare agents (CWA's) and simulants on surfaces. Real CWA's are far too dangerous for experimental study in any but a small number of specially-equipped facilities, which limits the rate at which such compounds can be investigated and characterized. Most exploratory work on CWA detection and remediation is done using simulants, i.e., species which are safe enough for routine handling and which (it is hoped) behave in a manner closely similar to real CWA's. It is often not possible to compare directly the simulant and the corresponding CWA, again because of the difficulties inherent in working with the latter. Thus, it is often not possible to evaluate the degree to which the simulant mimics the properties of the real CWA in a particular type of measurement. *Ab initio* quantum-chemical theory can relieve much of the burden of working with real CWA's through the use of modeling. The focus of the current work is on the adsorption of a CWA (Sarin) and a simulant (DMMP) on an oxide (γ-Al_2O_3). The results obtained to date show that adsorption results for large, but free-standing, cluster models (i.e., $Al_{20}O_{30}$) are in quantitative agreement with experiment. It is also found that the structure and energetics of adsorbed DMMP closely resemble those of Sarin, verifying that DMMP is a reliable simulant for the real CWA.

Significance: The work on β-Ga_2O_3 is the first *ab initio* theoretical study of the surface of this material. This is, to date, the only analysis (either in theory or experiment) of the structure of different β-Ga_2O_3 surfaces. The CWA studies are the first to report a "side-by-side" comparison of the adsorption behavior of a simulant and the corresponding real CWA.

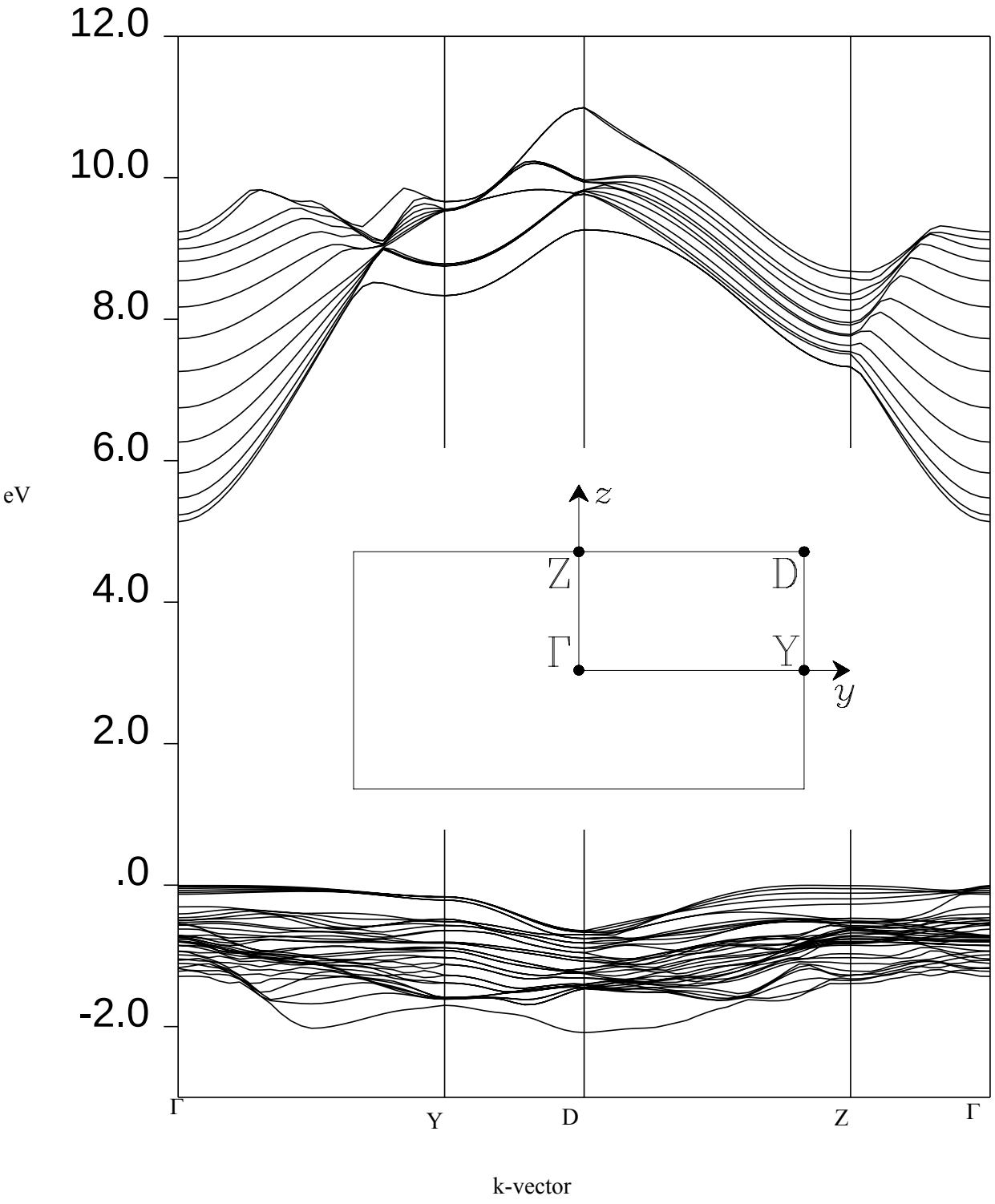


Figure 1. Surface band structure diagram, computed using DFT with the B3LYP functional and all-electron basis sets, for the fully-relaxed (1 0 0)-B surface of β-Ga_2O_3. The inset shows the surface Brillouin zone. The region shown comprises the upper (lower) part of the valence (conduction) band, and the zero of energy is at the valence band maximum. The y-axis lies parallel to the [0 1 0] direction.

Title: Multiple Length and Time Scale Simulations of Material Properties
Author(s): N. Bernstein
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

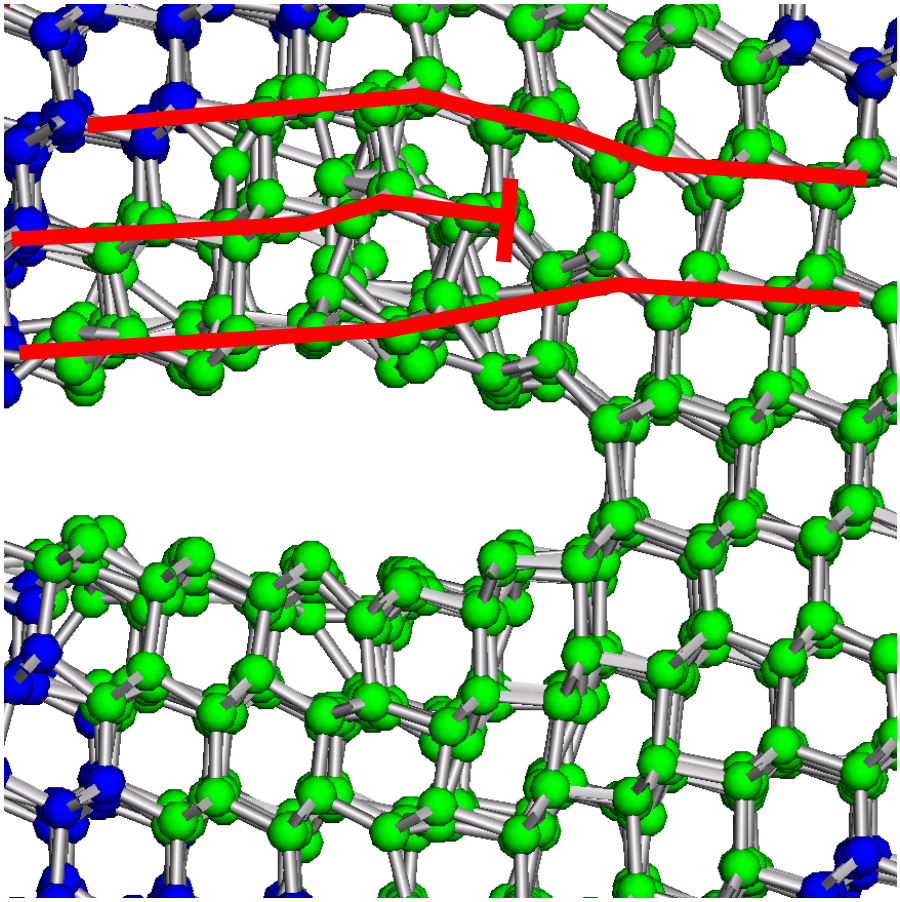
Computer Resources: Linux Networx Xeon Cluster [ARL, MD]; HP Opetron XC, SGI Altix [ASC, OH]; Cray XT3 [ERDC, MS]; Cray XD1, SGI Altix [NRL, DC]

Research Objectives: To understand and predict mechanical and structural properties of materials using atomistic and coupled computer simulations.

Methodology: We use several methods to simulate mechanical properties, including large scale molecular dynamics (MD), tight-binding quantum-mechanical models, *ab initio* density functional theory, and methods that couple multiple computational approaches. Tight-binding (NRL-TB, parallelized using MPI) and density-functional theory (VASP, parallelized using MPI) calculations are used to study material properties that control fracture and plasticity in silicon carbide. Tight-binding molecular dynamics (NRL-TB) is used to simulate the annealing of amorphous silicon. Tight-binding MD coupled dynamically to empirical potential MD (parallelized using mixed MPI/OpenMP) is used to study fracture in insulators.

Results: Simulations of fracture in silicon at high temperatures were carried using a coupled quantum-mechanical and interatomic potential molecular dynamics method. Extended duration runs of a long strip with a pre-crack were carried out, and a transition as a function of temperature was observed. At $T = 900$ K, fracture was brittle and the crack remained sharp. At $T = 1000$ K, dislocations were observed nucleating from the crack (visualization in attached graphic). Analysis indicated that these were shuffle-set dislocations, which are only mobile at high applied stresses. As the crack continued to advance, the dislocations are annihilated at the exposed surface. Using tight-binding molecular dynamics we annealed a sample of amorphous silicon for over 1 ns. This time scale, previously reached only with interatomic potentials, made it possible to create a sample that reflects the energetics of the more reliable tight-binding model, rather than the initial structure which originated from an interatomic potential simulation. The final structure has a radial distribution function that is in excellent agreement with experiment, in contrast with most previous results that have a first-neighbor peak that is double the experimentally observed width. Further, the annealed structure shows coordination defects, despite having a lower total energy than the initial structure, suggesting that the lowest energy amorphous structure *may not be* a perfectly four-fold coordinated continuous random network. To prepare for simulation of fracture in silicon carbide, we carried out a study of surface energies and generalized stacking-fault energies. In addition to the elastic constants, these are the essential parameters that control the fracture and plasticity in crystalline solids. We used *ab-initio* density-functional theory calculations to establish baseline values for energies of several high-symmetry surfaces and unstable and intrinsic stacking fault energies for several inequivalent (111) slip planes. Comparison to tight-binding calculations of the same quantities shows that the NRL-TB model is good in most cases, but that additional fitting will be needed to correct the energetics for some surface orientations.

Significance: Amorphous silicon is closely related to hydrogenated amorphous silicon, a material with applications in inexpensive electronics and photovoltaics. Our simulations directly contribute information about the structure, and assist analysis of experimental probes such as diffraction spectra. Fracture is an important mechanism for mechanical failure for structural materials. Silicon is a model system for materials with a temperature dependent brittle to ductile transition, and our coupled simulations are revealing how this transition is initiated on the atomic scale. Silicon carbide is an important material for applications ranging from MEMS to body armor SAPI plates. A reliable tight-binding model of SiC will enabled coupled simulations of fracture that will show how failure occurs in polycrystalline samples.



Coupled tight-binding (green atoms) and interatomic potential (blue atoms) simulation of fracture in silicon at T=1000 K showing a dislocation nucleated at the crack tip. Red lines indicate atomic planes.

Title: Molecular Dynamics Simulation Studies of Intra- and Intermolecular Forces in Biological Systems
Author(s): Jeffrey Deschamps[1] and Alexander D. MacKerell, Jr.[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]University of Maryland, School of Pharmacy, Baltimore, MD
CTA: CCM

Computer Resources: COMPAQ SC40/45, SGI Origin 3000 [ASC, OH]; SGI Altix [NRL, DC]

Research Objectives: Molecular dynamics (MD) and quantum mechanical (QM) theoretical approaches were applied to obtain atomic details of the relationship of structural and dynamical properties to activity and reactivity of biological molecules, including opioids, proteins, DNA, RNA and lipids.

Methodology: QM and MD methodologies were used to study the chemical, structural and dynamical properties of selected molecules. QM studies were performed using the Gaussian suite of programs with optimizations performed to default tolerances. Access to DFT treatment of electron correlation allowed for *ab initio* methods to be applied to the opioids. MD simulations were performed using the program CHARMM with empirical force fields developed as part of our ongoing research program. CHARMM runs in parallel on the Compaq, SGI and Cray XD1 architectures using MPI. Empirical force field development used *ab initio* data that included explicit treatment of electronic polarization. MD simulations were performed with an explicit solvent representation, including counterions, in the presence of either periodic boundary or stochastic boundary conditions. Free energies associated with the base flipping process were obtained via potential of mean force calculations, where the sampling is performed via MD simulations.

Results: Advances continued to be made in empirical force fields as well as in our studies of protein, DNA, RNA and opioid structure-function relationships. In the area of force field development tests of the CMAP extension of the CHARMM22 all-atom additive protein force field showed the model to improve the treatment of protein dynamics. Force field development with respect to the polarizable force field involved advances in optimization of a new water model and in the extension of the model to include an anisotropic electrostatic model based on a combination of lone pairs and anisotropic polarization on hydrogen bond acceptor atoms. The inclusion of these terms was shown to give a significant improvement in the balance of interactions of hydrogen bond acceptors with their environment. Progress was also made in the area of base flipping. This included identification of the range of flipped states that are actually observed in NMR experiments based on imino proton exchange. In addition, the role of different dihedrals in the phosphodiester backbone in base flipping was quantified. In another area of interest, we have successfully applied computer-aided drug design approaches to identify inhibitors of the signalling protein ERK that functions via protein-protein interactions.

Significance: Empirical force field based studies of macromolecules continues to grow as a field, with the developments in our laboratory positively impact the applicability of the method via significant improvements in accuracy. Such improvements will facilitate theoretical studies of a wide range of both biological and non-biological systems such as protein-protein interactions that are essential steps in cellular signal transduction pathways and the specificity of DNA-protein interactions that are essential for gene transcription and DNA repair. Of particular importance in the area of DNA-protein interactions is the conformational change in DNA referred to as base flipping. Our studies in this area have yielded insights into the energetic determinants of base flipping with respect to the methlation of cytosine bases, a phenomena which plays a role in gene regulation and in epigentics.

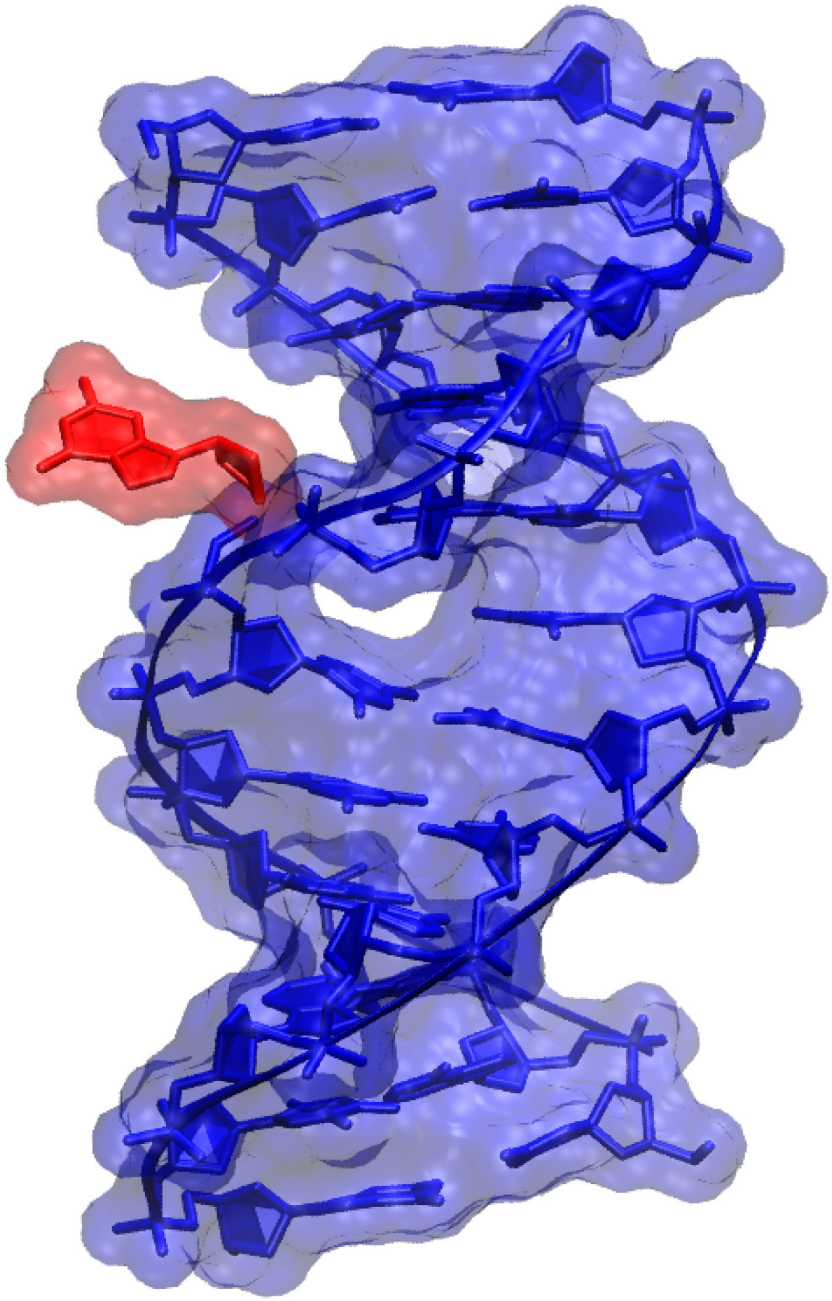


Image of a DNA duplex with a single guanine nucleotide (red) flipped out of the duplex structure. Structure obtained from U. D. Priyakumar and A. D. MacKerell, Jr., "NMR Imino Proton Exchange Experiments on Duplex DNA Primarily Monitor the Opening of Purine Bases," *Journal of the American Chemical Society* 128:678-679 (2006).

Title: Quantum Information Processing
Author(s): C. Stephen Hellberg and Kristopher E. Andersen
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

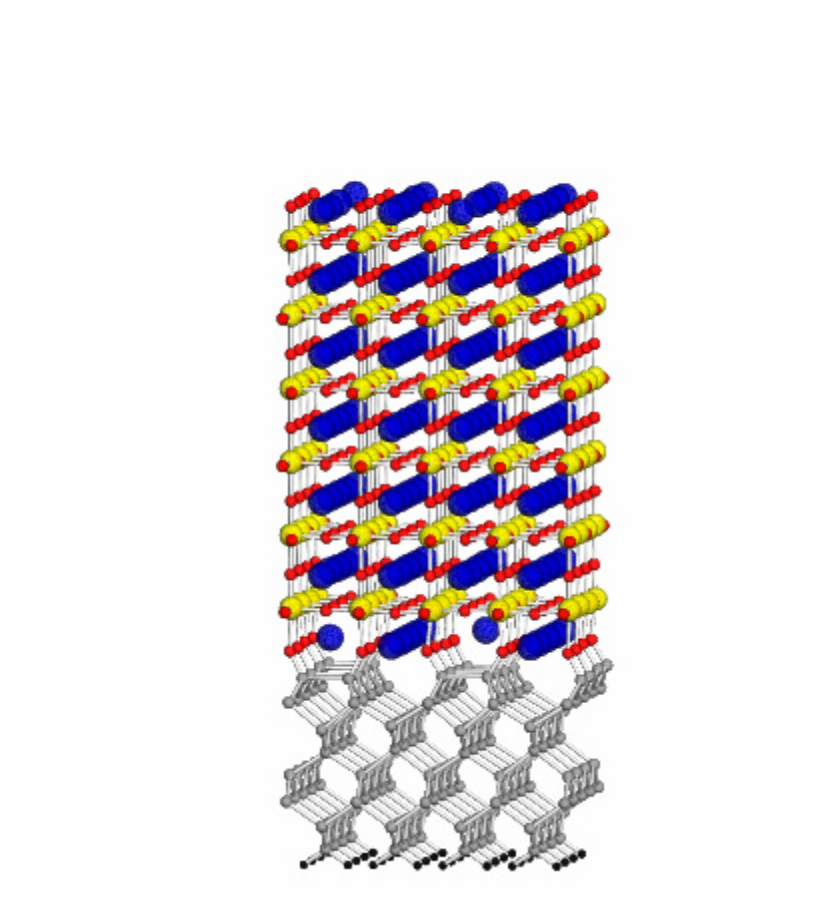
Computer Resources: SGI Altix, HP XC [ASC, OH]

Research Objectives: To improve the growth of $SrTiO_3$ on Si. There has been great interest in growth of complex oxides on silicon for device applications. $SrTiO_3$ has served as the prototypical system, but initial optimism has faded somewhat as well ordered epitaxial films have been difficult to achieve. Recently there have been several developments that have dramatically improved our understanding of these systems. Growth of coherent lattice-matched films has finally been achieved (but only for films 5 monolayers thick), and the measured expansion of the out-of-plane lattice constant exceeds the prediction of the bulk elastic constants of $SrTiO_3$ by nearly 100%. Simultaneously, growth by a different process in thermodynamic equilibrium yields islands of $SrTiO_3$.

Methodology: We used first-principles density functional calculations to determine the ground state structure and polarization of $SrTiO_3$ grown on Si. We first used the VASP planewave code at the ASC HPC center. This code allows a system with many atoms (we used up to 332 atoms) to be simulated and, most importantly, relaxed accurately.

Results: We showed that the energetically favored structure of $SrTiO_3$ on Si is one that has never been considered before and has a charged interface. We find the charged interface is favored for the entire allowable range of chemical potentials of the constituent atoms. The new structure agrees well with X-ray diffraction and absorption measurements on five-monolayer films. The polarized $SrTiO_3$ partially screens the field between the positively charged interface and negatively charged surface, but a strong electric field remains. As the film grows thicker, its energy can be reduced by ionic diffusion from the interface to the surface to reduce the field. Thus the favored structure changes as a function of film thickness, and the films are unstable to phase separation, which has been observed in scanning transmission electron microscopy experiments on films grown in thermodynamic equilibrium. It is argued that the kinetic barriers to ionic diffusion will eventually make non-equilibrium layer-by-layer growth unstable to "catastrophic roughening".

Significance: There has been great interest in growth of complex oxides on silicon for device applications, with functionality beyond standard CMOS technology. $SrTiO_3$ has served as the prototypical system, but initial optimism has faded somewhat as well ordered epitaxial films have been difficult to achieve. Our results show why it is so difficult to grow well ordered films. Most importantly, by understanding the cause of the disordered films, namely the charged interface, we can explore ways to get rid of the interface charge, and we are currently working in this direction.



Energetically favored structure of a 6 monolayer film of $SrTiO_3$ on Si(001). The cell has $\sqrt{8} + \sqrt{8}$ periodicity. The bottom Si surface is terminated wth hydrogen. There are ⅝ monolayers of Sr at the interface and ⅞ monolayers of Sr at the surface, resulting in an electric polarization of p = ¼ and enhanced *c/a* ratio as observed in experiments.

Title: Computer Simulation Modeling of Fluid Flow Through Porous Media
Author(s): J. F. Gettrust[1] and R. B. Pandey[1,2]
Affiliation(s): [1]Naval Research Laboratory, Stennis Space Center, MS; [2]Department of Physics and Astronomy, University of Southern Mississippi, Hattiesburg, MS
CTA: CCM

Computer Resources: IBM P4 [NAVO, MS]

Research Objectives: Continued efforts are made to understand the morphological (structural) evolution and flow (dynamics) of complex fluid mixtures in matrix media suitable for ocean (geomarine) environment using computer simulation models. Parameters affecting the flow, phase changes, and structures are, composition and distribution of the sediments, characteristics of fluid constituents, i.e., interactions and miscibility, concentration, temperature, pressure gradients, flow field, etc. Major questions we address are, how do density profiles evolve? How do flow rates of constituents depend on these parameters? Where does the linear response of flux rate, i.e., the Darcy's law apply and where does it fail? How do different phases (solid, liquid, gas) emerge and how do they depend on these parameters? We understand some of these questions for simple one component in an effective medium with our model. Challege remains to understand these questions for the multi-component systems by systematic computer simulation studies.

Methodology: We use the idea of Monte Carlo and lattice gas methods to study the fluid flow through porous media. The porous medium is modeled by direct simulation methods to incorporate structural morphology and appropriate porosity. The fluid is represented by particulate constituents with appropriate characteristics which include interactions and molecular weight. Predicting the complete response (linear and nonlinear) properties in such a complex system emerging from the basic constitutive details incorporated in the beginning of simulations is one of the major advantages of our approach.

Results: Density and velocity profiles, correlations, and flow of fluid through an open porous medium is studied on a three dimensional lattice. The bottom of the lattice is connected to a source while the top is open. We have studied in detail the response of flow rate and density profiles to concentration gradient, pressure gradients, temperature, porosity, etc. in an interacting, monodisperse lattice gas in porous media. In recent years, we have reported a number of interesting findings on linear and non-linear responses and density profiles as a function of these parameters. We have also studied the structure and dynamics of miscible fluid mixtures and found an exponential density decay with the height and a power-law dependence of the flux rate density on the porosity. These studies are extended to immiscible fluid mixtures with different molecular weights: a multi-phase system emerges in the steady-state, a dissociating solid phase from the source is separated from a migrating gas phase toward top by an interface of mixed (bi-continuous) phase. Scaling of solid-to-gas phase with the altitude is non-universal and depends on both the range of the height and the magnitude of the pressure bias. Onset of phase separation and layering is pronounced at low bias range. Currently, we are studying the response of flow, phase changes (pattern formation) and phase separation to pressure bias for a range of molecular weights of the constituents.

Significance: The problems of flow in heterogeneous systems are complex and lack appropriate laws and predictions. Our computer experiments make specific predictions for density profile and flow rate of gas (applicable to the dissociation of methane hydrate). Measuring the dissociation of methane hydrate within sediments and understanding its distribution and flow are difficult issues in field measurements but very important to some of the Navy projects that are being carried out here. In the absence of systematic field observation, our computer simulation studies provide an understanding of how methane gas flows and is distributed in porous media in appropriate physical (parametric) conditions. These studies also help advancing the frontier of knowledge in issues crucial to NRL as well as to understanding of science.

CEA

Computational Electromagnetics and Acoustics

- High-resolution, multidimensional solutions of Maxwell's equations to define the electromagnetic fields about antenna arrays; electromagnetic signatures of tactical ground, air, sea, and space vehicles; electromagnetic performance and design factors for EM gun technology; electromagnetic signature buried munitions; high-power microwave performance; and interdisciplinary applications in magnetohydrodynamics and laser systems.

- High-resolution, multidimensional solutions of the acoustic wave equations in solids, fluids, and gases to model the acoustic fields for surveillance and communication, seismic fields for mine detection, and the acoustic shock waves of explosions for antipersonnel weapons.

Title: Calculating Higher Order Statistics of Ocean Environmental Scattering and Reverberation
Author(s): Kevin D. LePage
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: Linux Cluster [SMDC, AL]

Research Objectives: The higher order statistics of bottom scattering and reverberation will be estimated through Monte-Carlo techniques and closed form theory in order to determine the non-Rayleighness and associated probability of false alarm for sonar systems as a function of system characteristics, background waveguide properties and scatterer distributions.

Methodology: We propose to exercise models developed at NRL and SACLANTCEN for the prediction of time series scattered from complex multi-layered sediments over ensembles of expected bottom variability. We propose to continue the investigation of the non-Rayleighness of scattering and reverberation initiated in FY05, exercising the models for non-Gaussian distributions of scatterer height, sound speed, and density contrast. Results from FY05 show that scattering and reverberation can be highly non-Rayleigh for sufficiently small patch sizes and negligible multipath. These results were obtained using the highly accurate NRL/SACLANTCEN models on the HPCMP resources for a limited number of scatterer distibution scenarios. In FY06 results will be generalized for a variety of realistic shallow water reverberation scenarios.

Results: Results in FY06 showed that it was possible to model the observed clutter characteristics of reverberation measured on the Malta Plateau south of Sicily using the measured background characteristics of the waveguide, including range dependent bottom and subbottom bathymetry. Results were reported at conferences and in the literature.

Significance: The current generation of tactical decision aids has been criticized for providing estimates of system performance under the assumption of Rayleigh reverberation. The work described above will support the eventual inclusion in these systems of more accurate estimates of the probability of false alarm.

Title: Large-Scale Computational Electromagnetics
Author(s): Richard S. Schechter, Mark Kragalott, and Michael S. Kluskens
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: SGI Altix [ASC, OH]; IBM P4 [ARL, MD]

Research Objectives: The objective is to use large-scale simulations of electromagnetic wave propagation to model such problems as the performance of complex antenna arrays and their radiated fields. Large-scale implies 3D modeling of a complete antenna or element in great detail and with enough surrounding free space by using a very large computational grid. This necessitates the use of large computers with many processors. Another objective is to improve the accuracy and fidelity of these simulations by devising more accurate algorithms and testing them against benchmark or known solutions.

Methodology: The finite-difference time domain (FDTD) technique is a widely used method in computational electromagnetics. The method is well suited for modeling wave propagation in heterogeneous media and scattering.

Results: Methods of modeling left-handed materials and their applications are now being studied. FDTD modeling of a left-handed materials (LHMs) composed of split-ring resonators (SRRs) and wires on circuit boards has been successfully accomplished. In a certain narrow band of frequencies, the material becomes left-handed. This has been proven conclusively by modeling cw waves propagating through a wedge-like structure composed of circuit boards with SRRs and wires. In a certain band of frequencies, the wave fronts bend to the opposite side of the normal as predicted by Snell's law. Outside of this band, the material is right-handed. This is vividly demonstrated by computational snapshots of the wave fields. It is hoped that applications to antennas or lenses can be found. An MPI computer code (CFDTD) has been successfully ported to a large HPC SGI Altix Linux machine. This FDTD code is special since it uses a contour method to model a curved structure, which it meshes, and non-uniform gridding. The code is now being used to model a large complex Vivaldi array antenna using more than a billion cells. This scalable FDTD code will be useful in the future for modeling electrically large structures requiring many processors.

Significance: In LHMs, electromagnetic waves have negative phase velocity and have been found to make superior lenses. LHM structures also have very useful properties for a variety of applications in communication, radar, sensor and optical signal generation and processing. Large phased array antennas and improving their performance is important to the Navy.

Title: Three-Dimensional Elasto-Acoustic Modeling
Author(s): Luise S. Couchman[1] and Saikat Dey[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]SFA Inc., Crofton, MD
CTA: CEA

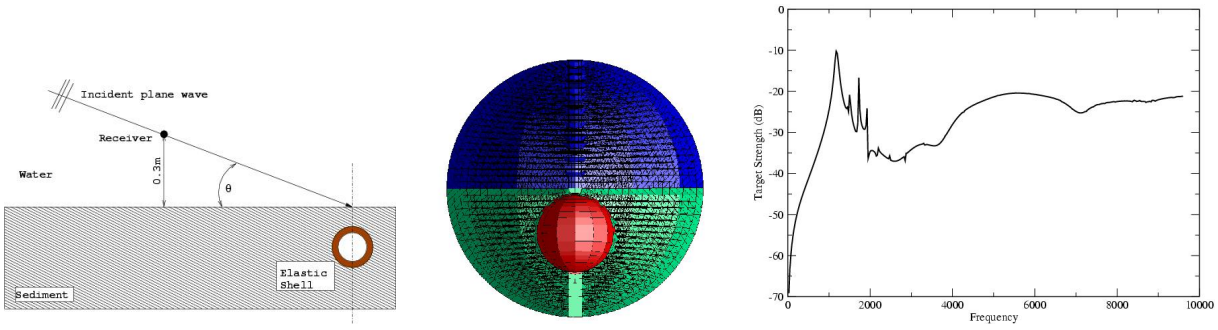
Computer Resources: SGI Altix, Cray XD1 [NRL, DC]; IBM P4 Linux Networx Cluster [ARL, MD]

Research Objectives: Numerical modeling of large-scale structural-acoustics problems using STARS3D. Applications include radiation and scattering from complex elastics structures; scattering in littoral environment using a two-fluid model.

Methodology: STARS3D utilizes hp-finite element approximations providing high accuracy solutions for mid-to-high frequency domains. Homogeneous infinite exterior medium is handled using infinite elements while inhomogeneous infinite exterior is modeled using perfectly matched layer (PML) technique. Scalable parallelism is natural for multi-frequency solves. Single-frequency solutions utilize domain decomposition (FETI-DP) algorithm. Parallel implementation is realized using MPI.

Results: Figure 1 depicts the case of modeling scattering from an elastic sphere near the fluid-sediment interface in a littoral environment. The sediment is treated as another damped acoustic fluid.

Significance: 1) The scalable performance and accuracy afforded by STARS3D is enabling scattering and radiation simulations for increasing complex targets. It also enables reliable results at increasingly high wavenumbers. Numerical results produced by STARS3D are expected to act as baseline solutions for a set of benchmark problems in 3D radiation and scattering. 2) Accurate modeling of littoral scattering for 3D targets is critical for mine-countermeasure efforts as well as harbour-threat modeling and mitigation.



(a) (b) (c)

Figure 1. Scattering from an elastic spherical shell in sediment: (a) problem description, (b) finite element mesh and (c) computed target-strength.

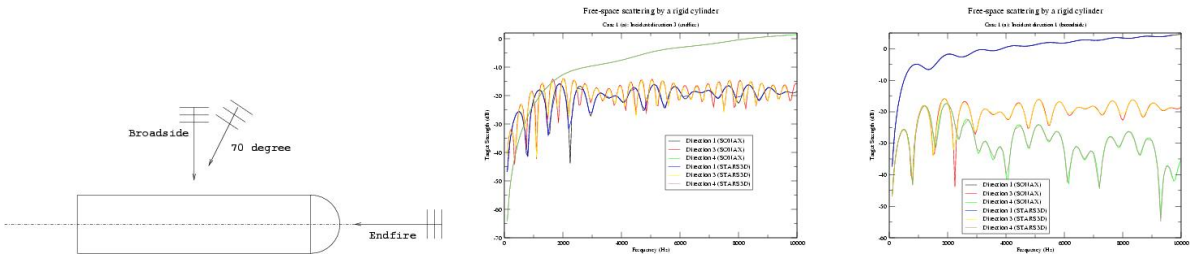


Figure 2. NURC benchmark problem: target-strength for endfire and broadside incidence.

Title: Influence of Near-Surface Bubbles on Acoustics
Author(s): Guy V. Norton
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CEA

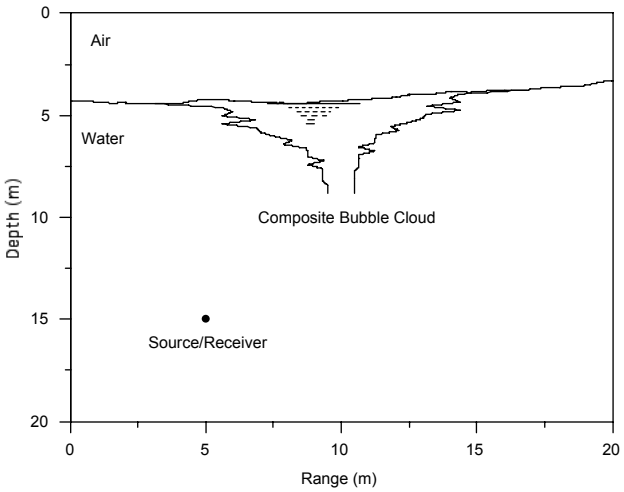
Computer Resources: SGI Altix [NRL, DC]

Research Objectives: Identify and quantify the dominant physical mechanisms that affect near-surface acoustic propagation and scattering in 3 dimensional/4 dimensional shallow water random media. Translate this knowledge of the dominant physical mechanisms into a strong, physics-based, performance prediction capability for acoustic systems in shallow water. Gain a deeper understanding of these physical mechanisms and understand the various coupling effects.

Methodology: Understanding how the sea-surface couples to the bubbles and affects the acoustic field will be determined. Numerical modeling will be performed to simulate the salt-water tank experiments and to include the simulated rough sea surface. This will allow for verification that the acoustic models have properly incorporated the essential physics (proper coupling of the rough surface with the bubbles). The results will be used in planning the at-sea experiments. Use highly accurate wave-theory supercomputer models (FEPE, FEPE-CM, FDTD with dispersion) to isolate/identify important physical mechanisms. Emphasize quantifying scattering, mode conversions, and resonances that occur immediately above and below the shallow-water ocean-surface interface, and on problems associated with application of lower-frequency full-solution models to high-frequency modeling (e.g., how to include effects of high-frequency absorption in the water).

Results: Using an acoustic model based on finite-difference-time-domain technique we have implemented a previously proposed theoretical technique to include both dispersion and attenuation directly in time domain calculation. Basic validation and verification of both the theory and numerical model has been accomplished. In addition this capability has been extended to two-dimensional heterogeneous dispersive media. A simulation in the time domain of both mono-static and bi-static scattered fields from a rough surface with a composite plume attached was performed. Results show that the received time series was significantly different than those modeled as non-dispersive (i.e., less reverberation). Additionally, each plume that made up the composite plume, acted on a different part of the signal due to its unique dispersive qualities. We developed FDTD models to solve the 2D heterogeneous and 3D homogeneous wave equation with dispersion.

Significance: The inclusion of dispersive effects directly in the time domain will provide a unique capability. It will allow for more realistic simulation of actual physical events that occur naturally during at sea experiments as well as during controlled laboratory experiments. This modeling capability is appropriate for determining the forward, and backscatter acoustic fields in 3 dimensions. Although the previously developed hybrid model known as EFEPE-CM correctly redistributes energy scattered from the rough sea surface and preserves the phase of the forward propagated field, (both of which the standard approximation of including surface roughness through a loss mechanism does not do), it is appropriate only for the forward field in two dimensions. It provides high fidelity calculations of the forward propagated field in the presence of a rough surface and a spatially, temporally and frequency varying ocean which is useful for simulations dealing with arrival structure and array signal processing where three dimensional effects are not important. Understanding the influence that these physical mechanisms have on mode coupling and on energy conversion will allow for the development of a sophisticated predictive capability. Other shallow water studies focus on frequency ranges that are of interest to low-frequency (1 Hz-1 kHz) or on active and weapons frequencies. This project spans the neglected range and includes the high-frequency range. The capability now exists to evaluate proposed experimental plans and to perform post-experimental analysis of collected data.



(Equation 1)

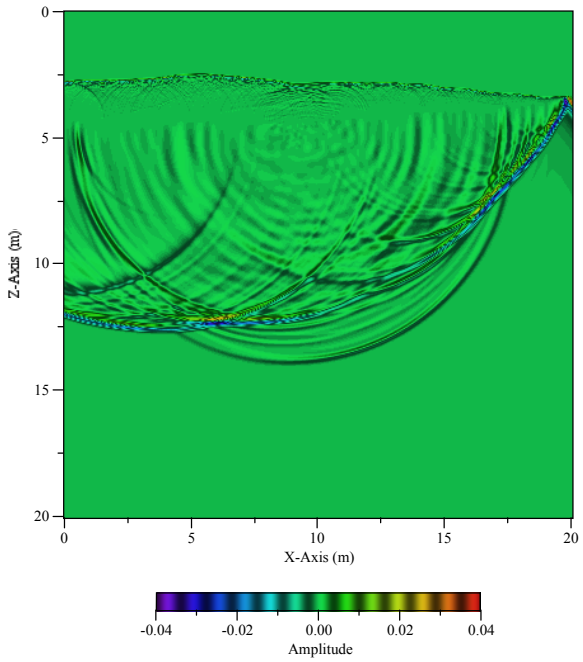
$$\nabla^2 p(r,t) - \frac{1}{c_0^2}\frac{\partial^2 p(r,t)}{\partial t^2} - \frac{1}{c_0}\frac{\partial\left(\Gamma(t) * p(r,t)\right)}{\partial t} = \delta(r - r_s)s(t)$$

(Equation 2)

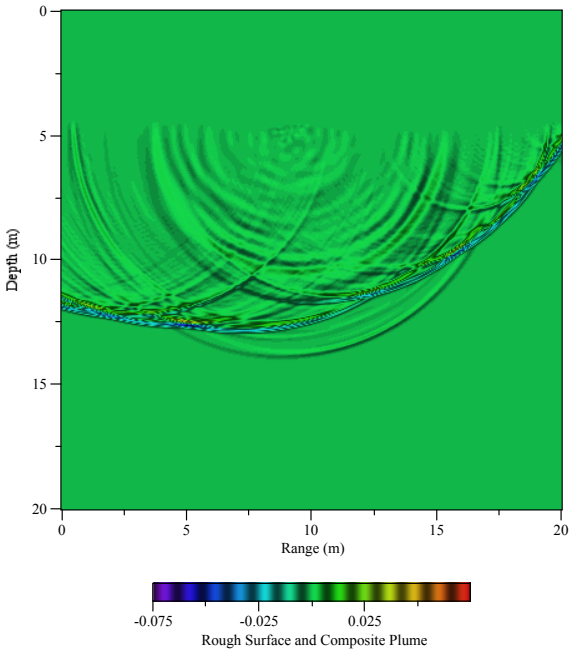
$$\frac{1}{\kappa(x,z)}\frac{\partial^2 u(x,z,t)}{\partial t^2} - \nabla \bullet \left(\frac{1}{\rho(x,z)}\nabla u(x,z,t)\right) + \sqrt{\frac{\rho(x,z)}{\kappa(x,z)}}\left(L_\gamma(t) * u(x,z,t)\right) = \delta(x - x_s)\delta(z - z_s)s(t)$$

Rough Surface with Composite Bubble Cloud

Homogeneous solution (Equation 1)



Heterogeneous solution (Equation 2)



Title: Dynamics of Coronal Magnetic Fields
Author(s): C. R. DeVore[1], S. K. Antiochos[1], J. T. Karpen[1], J. A. Klimchuk[1], M. G. Linton[1], B. J. Lynch[2], and B. T. Welsch[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]University of California, Berkeley, CA
CTA: CEA

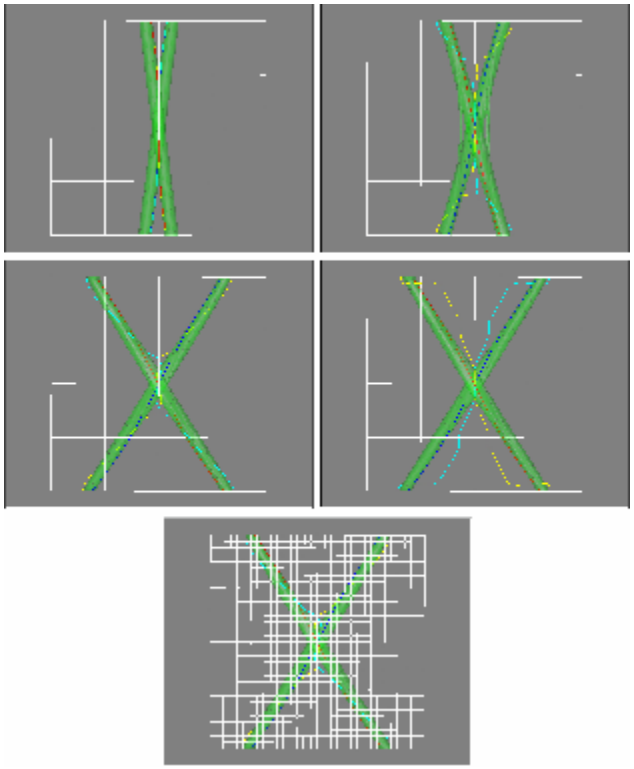
Computer Resources: Linux Networx Cluster [ARL, MD]; Cray X1 [ARSC, AK]; SGI Altix, SGI Origin [ASC, OH]; SGI Origin [ERDC, MS]; Cray XD1, SGI Altix [NRL, DC]

Research Objectives: Magnetohydrodynamic simulations were conducted on multiprocessor computers of the evolution of magnetic configurations that serve as prototypes for solar activity. The objective is to improve our understanding of the dynamics of solar magnetic reconnection, coronal heating, prominence formation, coronal mass ejections, and flux emergence. Resources also were used to enhance and test our state-of-the-art model for performing these complex simulations using adaptive meshing techniques.

Methodology: The numerical model, ARMS (Adaptively Refined Magnetohydrodynamics Solver), is a magnetohydrodynamics code that solves conservatively the evolution equations for mass, momentum, energy, and magnetic flux densities in three spatial dimensions and time. It uses a finite-volume formulation of the equations and flux-corrected transport (FCT) techniques to advance the variables. ARMS also employs techniques of adaptive mesh refinement, in which the grid adapts dynamically to the evolving solution for maximum efficiency and resolution. Our massively parallel implementation exploits distributed-memory systems via message-passing interface (MPI) communications.

Results: One of our investigations, newly launched this year, concerns the criteria for reconnection to occur between twisted magnetic flux tubes. This process is thought to be responsible for both confined (noneruptive) but violent solar flares and for gentler, episodic heating of the Sun's corona. Theory suggests that there is a critical angle between the magnetic field lines that must be reached before significant reconnection and energy release can occur. Previously, this problem has been addressed by simulations of continuous, volume-filling distributions of magnetic field. Our new approach instead uses discrete bundles of flux in the form of magnetic flux tubes, which are much more germane to the real coronal environment but are less well understood theoretically. The accompanying figure shows the result of an initial, exploratory simulation. Two straight flux tubes, illustrated by isosurfaces of magnetic field strength (*green*) and selected magnetic field lines (*red*, *blue*, *cyan*, and *yellow*), are initially slightly tilted with respect to, and separated from, each other (*top left*). They are subjected to motions applied at the top and bottom bounding planes that first gently bend the tubes around each other, and then gradually increase the tilt angle between them (*top right*, *middle left*). Field lines relatively deep within the tubes (*red* and *blue*) are not much affected except for being stretched out by the motions, while those near the surface of the tubes (*cyan* and *yellow*) undergo multiple reconnections in the current sheet formed in the contact region between the tubes, at the center of the images. Even after the footpoint motions have been stopped (*middle left* and *right*), the dynamical relaxation of the current sheet switches magnetic field lines back and forth (*cyan* and *yellow*) between the two flux tubes. The final image (*bottom*) illustrates the power of our adaptive mesh refinement algorithm, which refines the grid blocks (*white*) along the cross sections of the flux tubes and across the top and bottom bounding planes where the footpoint motions are imposed but coarsens them elsewhere, to maximize resolution while conserving resources.

Significance: Dynamical phenomena that affect the Earth and its near-space environment originate in the activity of magnetic fields in the Sun's corona. The Navy's interest in these matters stems principally from its reliance on space-based communications, navigation, and surveillance systems. Energetic particles and hard radiation also pose medical hazards to high-altitude pilots and astronauts in orbit.



Title: High-Accuracy Finite-Difference-Time-Domain Calculation of Electromagnetic Fields
Author(s): Michael I. Haftel
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: SGI Origin 3900 [ERDC, MS]; SGI Origin 3900 [ASC, OH]

Research Objectives: To develop the High Accuracy Scattering and Propagation (HASP) code for the 3D Maxwell's equations and to calculate the fields in and scattered from objects of naval or technological interest, including RF cavities and advanced materials.

Methodology: A highly accurate FDTD algorithm for solving Maxwell's equations (up to 10000 times more accurate than the Yee algorithm) is written into the HASP code. The algorithm has been implemented to take maximal advantage of parallel processing using Fortran 90. This code has been applied to calculating electromagnetic fields around and in complex 2D and 3D objects, including complex cavities and advanced materials such as photonic crystals.

Results: We used the HASP code to simulate the optical fields and optical transmission through nanoarrays of silica rings embedded in thin gold and silver films. A number of different ring geometries (inner and outer radii, film thickness, and periodicity) were simulated. The optical transmission spectra obtained for varying ring geometries uncovered large enhancements in the transmission at wavelengths much longer than obtainable for nanoarrays of similar cylindrical apertures. The computed field patterns in the apertures show that the enhancements are due to closely coupled cylindrical surface plasmons propagating on the inner and outer surfaces of the rings, and this coupling is more efficient as the inner and outer ring radii approach each other. The simulation results and their interpretation are consistent with the normal mode analysis of such structures. The behavior of the CSP dispersion is such that propagating modes can be sent through the rings for ever longer wavelengths as the ring radii approach, whereas the transmission decreases only in proportion to the ring area. The simulations were extended to metamaterials in the RF region, where similar results were obtained in relation to ring radii and film thickness. In this latter case the simulations confirmed that “spoof” CSP’s (i.e., surface waves) are generated by embedding a macroscopic periodic dielectric structure in a perfect conductor.

Significance: This work indicates how nanostructured arrays can enhance the optical properties of materials well beyond the diffraction limit. This will impact the design and performance of optical materials and devices used by the Navy for sensing and transmission. Also, these studies impact the design of metamaterials in the IR, microwave, and RF regimes for similar applications.

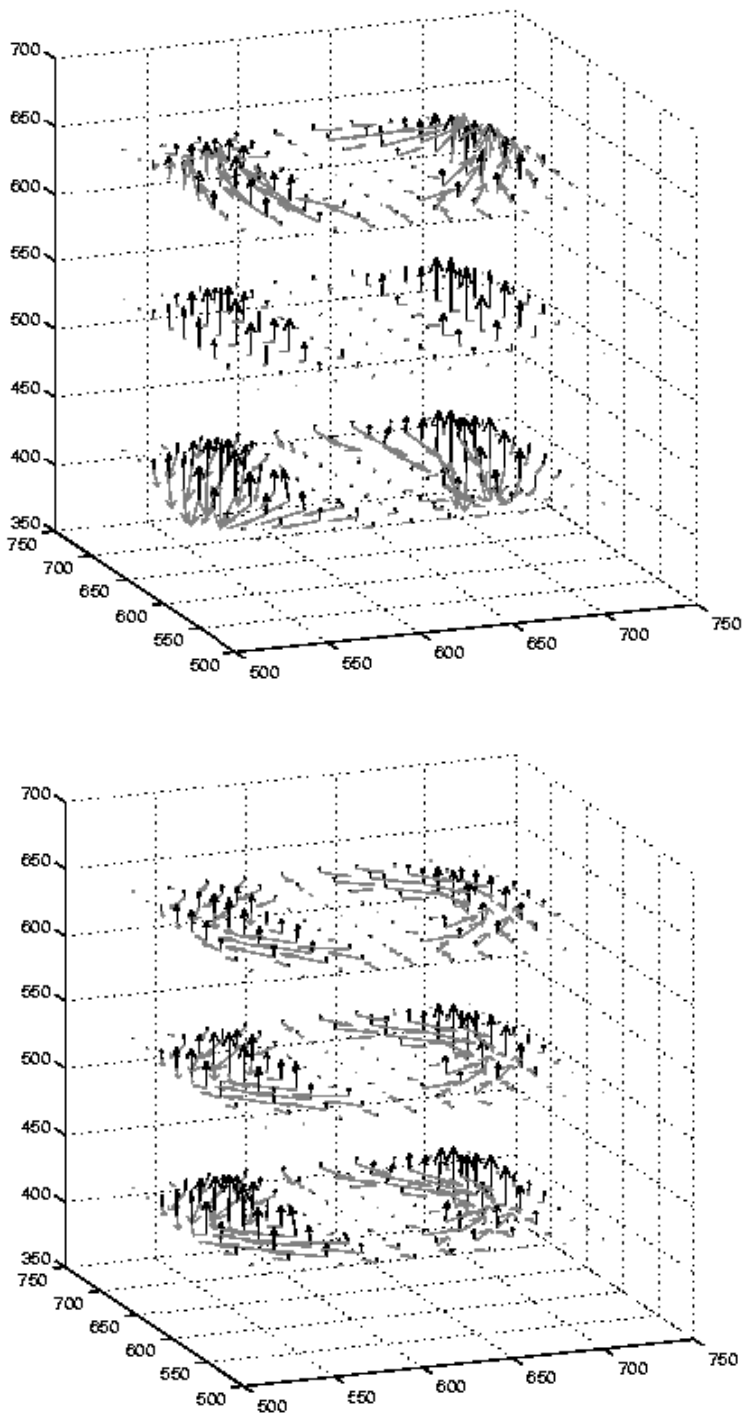


Diagram of the real (black arrows) and imaginary (gray arrows) parts of the Poynting vector in the coaxial ring aperture with inner and outer radii 50 and 100 nm respectively. The top is for $\lambda = 903$ and the bottom for $\lambda = 1000$ nm, which is the position of the cylindrical surface plasmon (CSP) resonance. Note the large imaginary part of the Poynting vector oriented azimuthally throughout the aperature in the bottom diagram, the signature of a CSP resonance.

Title: Infrasound Signal Propagation Modeling
Author(s): Douglas P. Drob, Joseph Lingevitch, and Geoffrey Edelman
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: Linux Networx Cluster [ARL, MD]; SGI Altix [NRL, DC]

Research Objectives: Advance the state-of-the-art in infrasound propagation modeling techniques to improve national/international capabilities to detect, locate, and characterize infrasonic signals and events. Utilize high-resolution, range and frequency dependent parabolic equation methods (NRL RAMPE) and acoustic ray tracing propagation codes to simulate and understand observed infrasonic signals produced by a variety of natural and man-made infrasound events, with particular emphasis on explaining the observed seasonal and local-time variations of recurrent volcanic infrasound signals in the south pacific.

Methodology: An initial effort is required to port existing NRL ground-to-space (G2S) global environmental specifications and infrasound propagation codes from single processor systems to HPC systems. These new codes will then be used to calculate the infrasound propagation observables from volcanic eruptions and other ground-truth events over a variety of geophysical parameter spaces (e.g., frequency, time, direction) into order to develop a better physical understanding of infrasound propagation and validate the computational techniques. Individual ground-truth events such as impulsive bolides, chemical explosions, and isolated volcanic eruptions, as well as three years of infrasound observations of daily eruptions of two volcanoes (Lopevi and Yasur) near New Caledonia will be considered.

Results: During the first year we successfully ported the G2S environmental specifications and NRL propagation codes to the HPC parallel/clustered systems. Application of these codes to a limited number of events and model parameter spaces has allowed us to initially validate the computational techniques. Figure 1 shows a 2D simulation of the acoustic radiation pattern from a bolide event that occurred over Washington State on June 4, 2003. The solid lines show the acoustic ray paths while the color image indicates signal attenuation at 1 Hz as predicted by RAMPE. In order to start to explore the role of daily and seasonal atmospheric variability on infrasound detectability for fixed source to receiver configurations we also performed initial calculations of Lopevi signal attenuation. Figure 2 shows the signal transmission loss at 1 Hz as function of range from the Lopevi volcano to the I57FR infrasound array located 648 km away, at 6 hour time intervals for 140 days in 2003.

Significance: This work will improved understanding of infrasound propagation physics over regional distances, including the effects of atmospheric variability, and provide new tools and techniques that improve national/international capabilities to detect, locate, and characterize clandestine nuclear explosions.

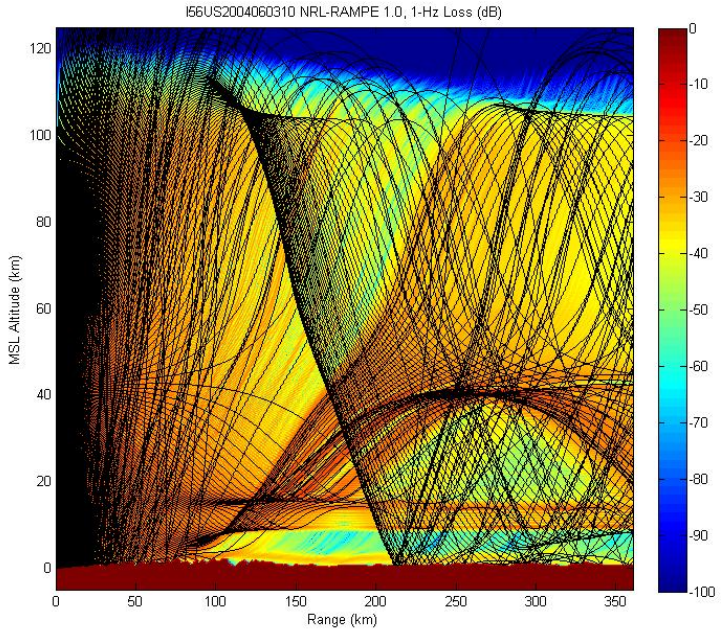


Figure 1. The 2D acoustic radiation pattern from a bolide event that occurred over Washington State on June 4, 2003. The solid lines show the acoustic ray paths while the color image indicates signal attenuation at 1 Hz as predicted by RAMPE.

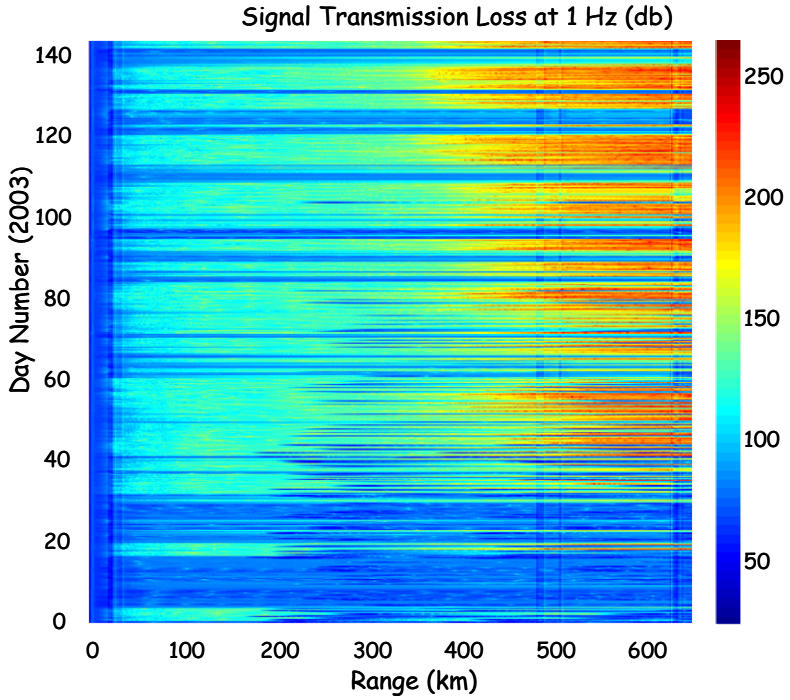


Figure 2. Signal transmission loss at 1 Hz as function of range from the Lopevi volcano to the I57FR infrasound array located 648 km away, at 6 hour time intervals for 140 days in 2003.

Title: Low Grazing Angle Radar Backscatter
Author(s): J. V. Toporkov and M. A. Sletten
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: SGI Altix [NRL, DC]; SGI Origin 3900 [ERDC, MS], [SMDC, AL]

Research Objectives: The purpose of this study is to gain and improve understanding of the behavior of ocean radar backscatter at low grazing angles (LGA) through direct numerical simulations of surface scattering processes. Sea clutter is often a significant factor in ship-borne radar systems. Various remote sensing applications use ocean backscatter as main source of information. Many of such systems operate in the LGA regime, and they all depend on the detailed knowledge of the sea clutter properties for their successful performance. However, the LGA sea backscatter exhibits rather complex features, many of which are still not well understood nor can be replicated with approximate scattering models. Direct numerical solution to the scattering problem allows detailed studies of ocean backscatter under controlled conditions of numerical experiment. The research focuses on the two electromagnetic frequency bands of primary practical interest: X band (wavelength 3 cm) and L band (23 cm).

Methodology: The technique combines an ocean surface model that includes non-linear hydrodynamics with computationally efficient, exact calculation of the electromagnetic backscatter. In this work, the wind-driven surface is represented by realizations of a Gaussian random process described by a certain model wave spectrum (Pierson-Moskowitz or Elfouhaily). The important short-scale roughness is shaped by wave-wave interactions modeled by the non-linear Creamer transformation applied to a Gaussian realization. The electromagnetic field scattered by a given surface profile at a particular frequency is found by iterating the second-kind integral equation for induced surface current. This technique is formulated from the first principles and, as such, automatically accounts for many phenomena (multiple scattering, shadowing) known to be problematic for analytical treatment. The numerical method shows robust convergence even as incident field direction approaches grazing. To simulate pulse scattering, surface response is calculated at a number of frequencies, and Fourier synthesis is used. Temporal evolution of a surface realization can be represented by a sequence of profiles, with scattering calculations repeated for each profile. Simulations are limited to a two-dimensional situation but have direct relevance to commonly occurring three-dimensional geometries.

Results: We continued the analysis the previously generated Monte Carlo data sets of range-resolved backscatter to evaluate correlation properties and probability density functions under different environmental conditions and system parameters, cf.. Figures 1 and 2. In addition to existing X-band sets, new data were generated at lower, L-band frequencies. Previous sets were also augmented with additional realizations to reduce statistical error in important probability distribution “tails”. One particular focus area was the sensitivity of results to the surface spectral model. It appears that replacing sophisticated Elfouhaily spectrum with its rather simplistic (and hence favored for analytical studies) Pierson-Moskowitz countepart results in only minor changes, with vertical polarization affected the most (Figure 1). Autocorrelation function of the range-resolved return appears to follow correlation function for the surface slope, with vertical polarization showing the best agreement (Figure 2). HPC resources were also used to process collected InSAR data and to produce velocity estimates for studied oceanic currents.

Significance: Detailed knowledge of the LGA sea clutter and of its dependence on environmental and other factors is essential for predicting and improving the performance of ship-borne radar systems and is vital for enhancing the quality of ocean-related remote sensing products. Direct numerical simulations replicate the input data as seen by such a sensor, establish correlations of these data with the wave fields being probed, and guide the development of advanced clutter models and data retrieval techniques.

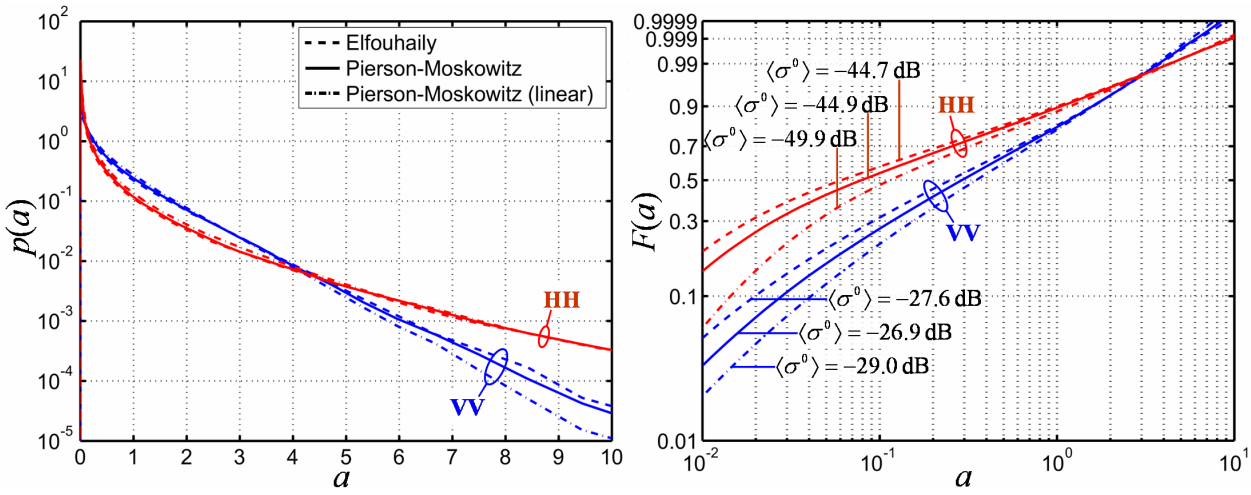


Figure 1. Comparison of surface clutter probability density functions (left) and cumulative distributions (right) for different surface models. A 2.2-ns X-band pulse incident at $\theta_i = 85^\circ$ is used. The wind speed $U_{10} = 4.73$ m/s in Elfouhaily spectrum matches the Pierson-Moskowitz parameter $U_{19} = 5$ m/s . By default, non-linear Creamer transformation is applied when either spectral model is used; the effect of turning this non-linearity off is also shown.

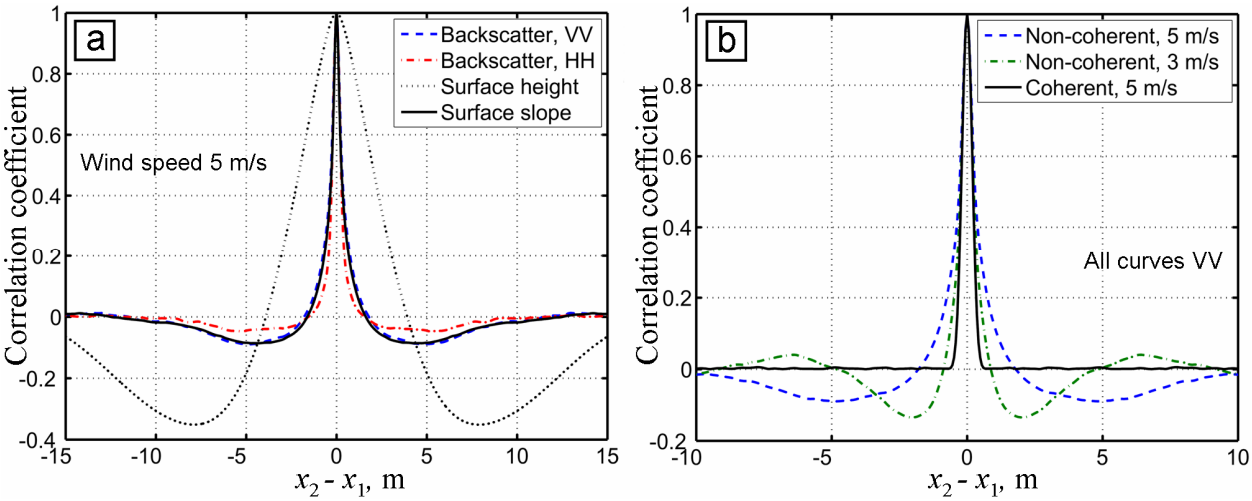


Figure 2. a) Correlation coefficients for non-coherent backscatter (i.e., signal magnitude) plotted along with their counterparts for surface height and slope. b) Correlation coefficients for non-coherent backscatter at different wind speeds, and an absolute value of the coefficient for coherent (complex amplitude) return. In all examples, a 2.2-ns, X-band pulse incident at 85° is used.

Title: Acoustic Error Modeling
Author(s): Josette P. Fabre
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CEA

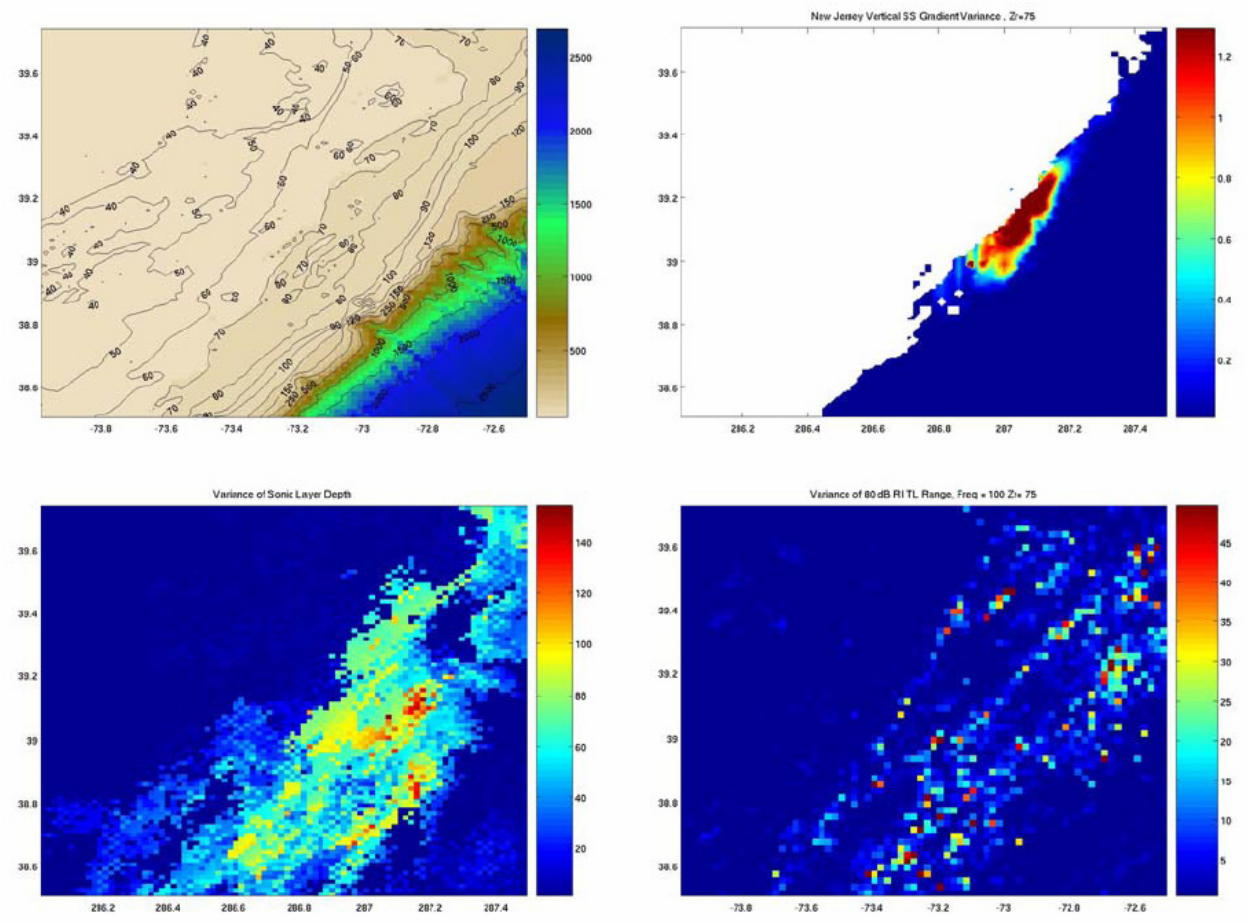
Computer Resources: IBM P4 [NAVO, MS]

Research Objectives: To quantify errors in acoustic fields based on errors in the input environmental fields, for example, sound speed, bathymetry, surface and sediment structure. This information will provide a valuable asset to both the operational and research communities providing uncertainty estimates of predicted acoustic fields. These uncertainty estimates will provide guidance on sampling (take measurements in areas of greatest error/uncertainty) as well as provide confidence in performance predictions. The current effort estimates error due to variations in the sound velocity field only. Ensembles of acoustic fields are computed based on oceanographic ensembles to describe acoustic error. This project includes visualization of the acoustic field as well as research into reduction in computation time based on the acoustic field properties. Now that the initial work has been proven successful, the project can be expanded to include error due to bottom and surface description(s). Additionally, these efforts will be expanded to support optimal search track planning and Tactical Decision Aid analysis.

Methodology: Several steps are taken to develop the capability described above. First, ensembles of oceanographic (sound speed) fields must be computed, this is done under a separate sub-project (NRLSS018). Next these fields are combined with bathymetry, sediment description and wind information to develop input files for the acoustic models. The development described here requires use of two acoustic propagation models: the Navy Standard Parabolic Equation (NSPE) model and the Kraken Normal Mode model. Both programs are single acoustic frequency wave propagation models that compute complex pressure and propagating normal modes respectively. Both programs also predict transmission loss (TL). These programs are written in Fortran and are not parallelized. However, for this project, each model must be run for each geographic position and for each frequency and source depth. This results in hundreds of thousands of runs. In order to maximize the computers capabilities the routine that creates the input files also creates a batch file for submission to the load leveler (LL) and shell scripts for assigning each serial job to a processor on the designated nodes. The LL script then submits each shell script to the Parallel Operating Environment (POE) and multiple serial runs are submitted in parallel.

Results: Several methods of estimating uncertainty due to the acoustic propagation have been developed for this task. These methods are currently being tested on the ONR SW06 being conducted off the coast of New Jersey. Maps of acoustic uncertainty due to sound speed uncertainty are being used to prepare glider measurement plans. Preliminary examples are given in the figure below.

Significance: In 2000, ONR initiated a program in this important area of research, uncertainty. Until recently, scarce measurements were input to models and the output was used for predicting the performance of a system. The prediction was not always accurate and the source of the error was unclear. The capability here directly addresses this problem by providing guidance for sampling strategies as well as providing variability (due to variability in sound speed only) of acoustic predictions.



Examples of acoustic variance for New Jersey exercise area. Top left shows the bathymetry, or bottom depth, of the area, top right shows the vertical sound speed gradient variance at a depth of 75m, bottom left shows the variance of the sonic layer depth (m) and bottom right shows variance of the range to which sound projected at 100 Hz from a depth of 25 m to a depth of 75 m will propagate to an 80 dB loss. As expected, the variance is greatest along the shelf break that runs from the lower left to upper right of each plot. These estimates are generated using ~24,000 acoustic propagation model runs which took approximately 60 minutes on 16 processors. The finalized program will typically use 500,000 runs per analysis area for acoustics alone (oceanography is being developed under a separate subproject).

Title: Intense Laser Physics and Advanced Radiation Sources
Author(s): Daniel F. Gordon and Richard F. Hubbard
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: IBM P3/P4 [MHPCC, HI], [NAVO, MS]; Cray XT3 [ERDC, MS]

Research Objectives: The primary objectives of this program are to model the propagation of intense, short-pulse lasers in plasmas and other nonlinear media, and to provide computational support for experiments on the NRL Table-Top-Terawatt (T^3) laser and Terawatt-Femtosecond-Laser (TFL). Current areas of research include plasma based accelerators, terahertz radiation generation, and laser guided discharge modeling.

Methodology: HPC resources are utilized using an object oriented parallel framework called turboWAVE which contains modules designed to solve a variety of problems. Both fully explicit and ponderomotive guiding center particle-in-cell modules are used to model relativistically intense laser pulses propagating in plasmas. Fluid modules are used to model atmospheric discharge physics. The framework supports non-uniform grids and sliding re-zones for problems with extreme space-scale separations.

Results: The SPARC module for modeling of laser guided discharges has been running in full production mode. SPARC solves the axisymmetric hydrodynamic equations for a multi-species plasma in combination with an electrostatic field solver and an air chemistry package. The primary achievement was modeling a lightning-like streamer over a propagation distance of 40 centimeters. Modeling streamer propagation over such long distances is notoriously difficult due to the disparate time and space scales involved. We solved this problem by combining a non-uniform grid and sliding re-zone with fully scalable parallelization. We also devised an efficient set of equations for modeling the electron transport. Our modeling also led to an important physical insight into the mechanism of leader propagation. In particular, using air chemistry models based on the assumption that the avalanche ionization rate depends only on the electric field and the neutral gas density was not sufficient to achieve long propagation distances. By relaxing that assumption (by keeping track of the nitrogen vibrational energy) it was found that a leader can form and extended propagation distances can result.

Significance: Laser-driven accelerators and radiation sources have potential applications for ultrafast (femtosecond) imaging of chemical and biological systems. The plasma-based pulse control methods currently being studied may be used to focus, shape, or compress laser pulses at intensities that are far above the limits of conventional focusing optics. Laser guided electrical discharges could have applications for non-lethal weapons or for mitigation of natural lightning.

CWO

Climate
Weather
Ocean Modeling

- Modeling of the Earth's climate and weather to improve scientific understanding of the oceanic and atmospheric dynamics and developing an oceanic and atmospheric prediction capability for both military operations (safety of flight, mission planning, optimal aircraft, ship routing, weapon system design) and civilian applications (fisheries forecasts, pollutant tracking, global change studies, and weather forecasts).

- Modeling of various properties of the ocean (temperature, salinity, currents) to improve the processing gain for acoustic antisubmarine warfare (ASW).

Title: Dynamics of Coupled Models
Author(s): John C. Kindle
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]; IBM P3/P4 [MHPCC, HI]; SGI Origin [ERDC, MS]

Research Objective: Investigate the coupling of dynamical ocean and atmospheric models. Provide a foundation for the development of scientifically valid, dynamically coupled atmosphere-ocean models.

Methodology: This project is a component of the NRL effort to develop a coupled ocean-atmosphere prediction system. The coordinated effort will address the basic and applied research, as well as issues in building and coupling the components of the system. Emphasis in this project will be on evaluating the quality of surface momentum and heat fluxes from the atmosphere model component of the Coupled Ocean-Atmosphere Mesoscale Prediction System (COAMPS) model, and studying the response of the Navy Coastal Ocean Model (NCOM) and Princeton Ocean Model (POM) to such surface forcing. Much of the project focus will be on the Pacific West Coast (PWC) region, one of the two primary test-bed regions for the development of the fully coupled COAMPS model.

Results: The nested high resolution model for the Monterey Bay (NCOM-ICON) has been tested and evaluated during upwelling and relaxation events observed in the Monterey Bay area. In collaboration with the 6.1 Core "Coupled Bio-Optical and Physical Processes" project, issues investigated during the past year include: coupling to the Navy atmospheric model COAMPS, NCOM-based model simulations on a curvilinear-orthogonal grid, use of sigma versus hybrid (sigma-z) vertical grids, coupling with a larger-scale model on the open boundaries, and bio-physical coupling in the NCOM-based ecosystem model.

The technology for the assimilation of glider data into the NCOM model has been developed. Based on the NCODA data assimilation system, the approach is being tested and evaluated with the assimilation of temperature and salinity data from a fleet of Slocum (WHOI) and Spray (SIO) gliders deployed during the ONR sponsored AOSN-II experiment in the Monterey Bay.

Additionally, a high resolution (~ 4 km) implementation of the regional NCOM-CCS model was accomplished in collaboration with the Dynamics of Coupled Models project. This implementation extends the domain to 52N and uses the DBDB2 2 minute bathymetry. In collaboration with the 6.2 NRL core project “CONESTS”, a comparable HYCOM model was implemented using the same domain, bathymetry and horizontal resolution.

Significance: Understanding and predicting the dynamics of the air-sea surface boundary layer is important for short and long-term weather forecasting. This is critical for operations and weapon deployment, especially in the coastal and littoral zones. Improved large to mesoscale forecast skill is critical to both military and civilian use of the oceans, particularly on the continental margins.

Title: COBALT
Author(s): John C. Kindle
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]; IBM P3/P4 [MHPCC, HI]; SGI Origin [ERDC, MS]

Research Objective: The primary objective of proposed research is to understand the physical dynamical influences on the biodynamical processes and optical properties of the North Pacific eastern boundary current regime.

Methodology: The project examines the dynamics of such California Current System (CCS) phenomena as the coastal jet, the undercurrent, the inshore countercurrent, eddies, filaments and meanders; the relative importance to these features of such forcing mechanisms as coastal upwelling, wind stress and wind stress curl, flow instabilities, coastal geometry, bathymetry and remote forcing will be investigated. Additionally, the impact of these dynamical features on the bio-optical processes operant in this coastal region will be examined. Temporal scales of interest range from synoptic to interannual.

The model domain extends from 30°N to 49°N and from the coast to 135°W with a grid resolution of 5 min. for the standard configuration. A 10 component ecosystem model is incorporated into the regional and sub-domain models.The high-resolution coastal model received boundary information from the global, multi-level NCOM model (1/8-degree grid resolution) that assimilates satellite altimeter data and MCSST observations.

Results: The nested high resolution model for the Monterey Bay (NCOM-ICON) has been tested and evaluated during upwelling and relaxation events observed in the Monterey Bay area. In collaboration with the 6.1 Core Air-sea coupling in the Coastal Zone project, issues investigated during the past year include: coupling to the Navy atmospheric model COAMPS, NCOM-based model simulations on a curvilinear-orthogonal grid, use of sigma versus hybrid (sigma-z) vertical grids, coupling with a larger-scale model on the open boundaries, and bio-physical coupling in the NCOM-based ecosystem model. In preparation for participation in the ONR sponsored Adaptive Sampling and Prediction (ASAP) experiment in the Monterey Bay in July-August of 2006, we developed a very fine resolution (with 500m resolution in the Bay) sub-model (called NCOM frsICON) of the Monterey Bay. The NCOM frsICON is coupled to the NCOM ICON model, and includes 9-component ecosystem model formulation. These models are currently being run in near real-time as part of the ASAP (Adaptive Sampling and Prediction) experiment.

A method for the assimilation of glider data into the NCOM model has been developed. And utilized in real-time. Additionally, a high resolution (~ 4 km) implementation of the regional NCOM-CCS model was accomplished in collaboration with the Dynamics of Coupled Models project. This implementation extends the domain to 52N and uses the DBDB2 2 minute bathymetry. In collaboration with the 6.2 NRL core project “CONESTS”, a comparable HYCOM model was implemented using the same domain, bathymetry and horizontal resolution.

Significance: The study of this eastern boundary current, a highly variable physically-forced system, will permit further development of predictive numerical models for the advancement of understanding of effects of various, large- and small-scale forcing on circulation patterns, coupled physical-biological dynamics and resultant bio-optical features across littoral transitions of the ocean.

Title: Coastal Relocatable Ocean Models
Author(s): Richard Allard, Dong Shan Ko, and Shelley K. Riedlinger
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]

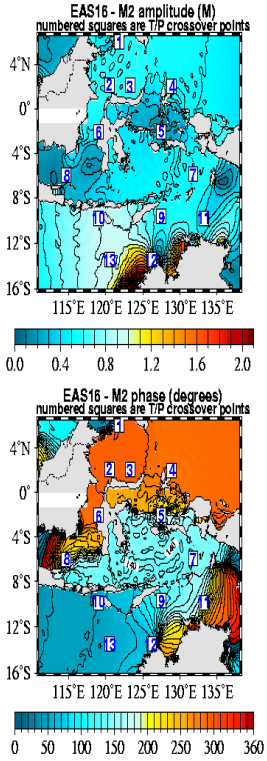
Research Objectives: To understand the processes which affect coastal and semi-enclosed seas through a combined use of ocean models, field observations and satellite data. The goal of this project is to use this understanding to develop state-of-the-art nowcast/forecast systems for Navy relevant coastal regions.

Methodology: Both Sigma- and Z- coordinate models as well as hybrid sigma/z coordinate models will be adapted to Navy relevant coastal regions. Several versions of the NRL Coastal Ocean Model (NCOM) and the Princeton Ocean Model (POM) have been applied to coastal and semi-enclosed seas of Navy interest such as the Mediterranean Sea, the Intra Americas Seas (IAS), the Yellow Sea/East China Sea, northern South China Sea and the East Asian Seas (EAS) region as well as the entire North Pacific basin. These models are driven by wind stresses and heat fluxes from the Navy Operational Global Atmospheric Prediction System (NOGAPS). The models are first developed and tested to prove that they can reproduce the general features of the ocean circulation. They are then further tested and validated against observations of temperature and ocean currents from sources such as XBTs and ADCP data. Once validated the models are delivered to Navy Operational Centers for final validation and then operational implementation. Planned upgrades to the relocatable system include a generalized vertical coordinate system that supports partial or "shaved" cells and a wetting and drying capability.

Results: The East Asian Seas Validation Test Report has been completed and submitted as an NRL Memorandum Report. The EAS river data base has been updated to increase the number of rivers from 51 to 139. Monthly river discharges at locations such as the Mekong River show much more realistic discharges with a maximum in August of 35,000 m^3/s versus the prior value of 5,000. Comparisons of the EAS tidal amplitude and phase for 13 TOPEX/Poseidon crossover points were made for the Indonesian Seas. The EAS rms error for amplitude was 3.9 cm and 17.3 for phase. One location was near a sharp gradient in bathymetry producing a 60° error in phase. When that point was removed, the rms error decreased to 4.4°. The Earth System Modeling Framework (ESMF) version of NCOM is being testing within EAS. The ESMF libraries are installed on the NAVO MSRC.

The 6.4 Small Scale Oceanography Project will deliver its baseline capability to NAVO by late September 2006. The system will be set-up with a series of scripts that generate bathymetry, tides, atmospheric forcing, initial and boundary conditions and climatological input fields.

Significance: The NCOM model has been successfully adapted to several coastal regions of Navy interest and has shown good skill in predicting the observed circulation. The high-resolution version of the EAS NCOM model, coupled to the Global NCOM is planned for a formal transition in FY07, while the relocatable modeling software will be transitioned into operational testing in early FY07.



M2								
			Amplitude (cm)			Phase (deg)		
Site #	LAT	LON	T/P	EAS	DIFF	T/P	EAS	DIFF
1	5.93	121.88	59.6	59.37	-0.23	290	292.36	2.36
2	2.15	120.47	58.9	58.95	0.05	290	294.88	4.88
3	2.03	123.28	57.2	57.03	-0.17	291	294.94	3.94
4	2.02	126.97	49.3	50.87	1.57	288	282.35	-5.65
5	-2.05	127.55	25.6	25.09	-0.51	160	163.31	3.31
6	-2.15	119.05	46.4	49.49	3.09	277	285.99	8.99
7	-5.9	131.82	58.5	51.12	-7.38	139	142.85	3.85
8	-5.97	114.8	13.4	19.8	6.4	140	200.47	60.47
9	-9.75	127.55	62.2	56.52	-5.68	120	117.64	-2.36
10	-9.75	119.05	83.1	88.71	5.61	54	51.01	-2.99
11	-9.77	133.22	43.5	41.52	-1.98	189	193.26	4.26
12	-13.5	126.13	84.7	85.47	0.77	62	61.86	-0.14
13	-13.52	120.47	89.7	94.48	4.78	56	51.63	-4.37
RMS	Difference: all sites			3.9			17.3	
RMS	Difference: excluding 8			3.6			4.4	

After Robertson & Ffield (2005)

Figure 1. (left) EAS M2 tidal amplitude (top) and phase (bottom) at the locations of TOPEX/Poseidon crossover points. The table on the right shows rms errors for amplitude and phase.

Title: Nearshore Wave, Tide, and Surf Prediction
Author(s): Richard Allard, Tim Campbell, James Dykes, Pam Posey, Erick Rogers, and Larry Hsu
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]

Research Objective: Provide the Naval Oceanographic Office the capability to produce 2-D surf and tidal predictions, including rip currents for littoral operations. Provide a reach-back capability for initialization fields produced at NAVO for the Mission Support Center. Support the Modeling & Simulation community by providing wave hindcast information for global and regional domains.

Methodology: Perform Wavewatch III hindcasts for a 10-year period (1993-2002) at a horizontal resolution of 0.1° for the Mediterranean Sea and Arabian Gulf. The WaveWatchIII spectra data can be used to provide spectral boundary conditions for regional SWAN wave model areas. PCTides has completed the documentation for the validation test report. It is anticipated that PCTides will formally be approved by the Administrative Modeling Oversight Panel (AMOP) in early FY07.

Results: 1) WavewatchIII was run for the period 1992-2001 to provide spectral boundary conditions for a SWAN Arabian Sea 10-year hindcasts. A new RTP "Smart Climatology" funded for FY06-08 required the running of WavewatchIII for spectral boundary conditions for a series of 3 SWAN nests for an area centered near the Taiwan Straits. Future efforts will require COAMPS, NCOM and SWAN hindcasts. A new HPC project "Smart Climatology" will address the ocean circulation and wave modeling beginning in FY07. 3) The PCTides Validation Test report was published as an NRL Memorandum Report in March 2006. The report provided information about the model physics, components of the PCTides2.0 system and several validation test cases. 4) The SWAN wave model has been configured into the ESMF superstructure where it at Level 4. Dr. Tim Campbell worked with a PET intern (Ben Payment) in implementing a parallel RESTART capability within SWAN. The ESMF version of SWAN will be tested with NAVO.

Significance: This research enhances the WSC's relocatable capability to run shallow-water wave, tide and surf models to support NAVOCEANO's contingency type oceanographic support for Naval exercises and operations.

Title: Atmospheric Process Studies
Author(s): Frank Giraldo, Tim Hogan, Young-Joon Kim, Justin McLay, Jim Ridout, and Carolyn Reynolds
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: Cray X1 [ARSC, AK]; IBM P4 [NAVO, MS]

Research Objectives: The research objective of this project is to develop and test a state of the art global data assimilation and prediction system that can be used to improve our understanding of the fundamental dynamical and physical processes that operate in the atmosphere. Specific tasks include extending the data assimilation and prediction system up to an altitude of 100km and improving probabilistic prediction.

Methodology: The Navy Operational Global Atmospheric Prediction System (NOGAPS) was developed for basic and applied atmospheric research and for operational numerical weather prediction. NOGAPS is continuously being upgraded through improving both the physical parameterizations and dynamical core, and NOGAPS serves as the modeling system that we use for our studies in this project. As part of this project, a new horizontal discretization method, the spectral element method, is being investigated as a replacement to the spectral transform method currently used in NOGAPS. Cloud-resolving simulations of convection are being run using the high-resolution Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS®[1]) to aid in physical parameterization development. New methods for ensemble design are being tested in order to provide improved probabilistic forecast. A portion of our work is also devoted to the use of simplified models to study exact solutions to problems not computationally tractable with complex operational models.
Results: Significant accomplishments were made in a number of areas. First, new orographic, convective, and spectral gravity wave parameterization schemes have been incorporated into the new NOGAPS-ALPHA (Advanced Level Physics and High Altitude) with a current top around 0.005 hPa (~85 km), producing comparable or better monthly climatologies and weather forecasts than the original NOGAPS system. The orographic gravity wave scheme has been further upgraded to include the effects of near-surface flow-blocking and orographic direction, and has been evaluated against explicit COAMPS simulations. The convective gravity wave scheme has also been upgraded to include the contribution from nonstationary waves in a simplistic, but computationally-efficient way. These can now be coupled to a spectral gravity-wave parameterization for the middle atmosphere, forming a self-contained scheme that does not require external wave source information – perfectly suited to real-time weather prediction. Second, new ensemble methods are demonstrably superior to the operational method in terms of ensemble mean error, spread-skill relationships, and other metrics, and should be transitioned to operations in FY07. The use of stochastic perturbations in ensembles has a significant impact on tropical cyclone track ensemble spread. Third, an improved representation of convective sensitivity to moisture variability is being developed for the Emanuel convective scheme in NOGAPS. Preliminary experiments suggest that the new treatment may significantly improve ensemble performance in the Tropics.

Significance: The continued development of the global model will have a significant impact on weather forecasting and will also aid in the advancement in understanding the physical processes in the atmospheric system. Improvements to the computational efficiency on distributed memory machines will greatly facilitate future computationally intensive forecast capabilities, such as ensemble forecasting. We expect that the extension of NOGAPS to 100 km will improve tropospheric prediction, as well as provide improved forecast guidance in the middle atmosphere. Improvements to the Navy ensemble forecasting system will significantly increase the utility of weather forecasts for the many users who need information on forecast reliability and uncertainty.

[1]COAMPS® is a registered trademark of the Naval Research Laboratory

Title: Coastal Mesoscale Modeling
Author(s): James D. Doyle
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: SGI Origin [ARL, MD], [ASC, OH], [ERDC, MS]; IBM P3/P4, Cray SV1 [NAVO, MS]

Research Objectives: Our objective is to develop and validate a coastal/littoral data assimilation and prediction system that can be used to provide high-resolution (<5 km) analysis/nowcast/short-term (0-48 h) forecast guidance for tactical sized areas of the world. This system can also be used for basic and applied research leading to an improvement in our understanding of atmospheric and oceanic processes. Further improvements to the mesoscale prediction system will result from the basic and applied research.

Methodology: The Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS®[1]) is being developed further for independent and coupled simulations of the atmosphere and ocean for the mesoscale. The atmospheric component of COAMPS is made up of a data assimilation system composed of the following elements: data quality control, multivariate optimum interpolation analysis, initialization, and a multi-nested, nonhydrostatic model. This model includes parameterizations for moist processes, surface and boundary-layer effects, and radiation processes. The NRL Coastal Ocean Model (NCOM) is currently being used for the simulation of the mesoscale ocean circulation response to the COAMPS forcing in one-way and two-way interactive modes.

Results: In FY06, COAMPS was demonstrated to be an accurate data assimilation and forecast system capable of predictions and simulations on a variety of scale from 0.3-9 km for land-sea effects and topographically driven flows. The dynamics of mountain-wave induced rotors were simulated over idealized mountain ranges with a grid increment of 60 m. These simulations reveal the presence of small-scale sub-rotor vortices that are suspected to be aviation hazards (Figure 1). High-resolution simulations of flow over terrain and mountain were conducted in conjunction with the Sierra Rotors Project (SRP) and the Terrain-Induced Rotors Experiment (T-REX), both of which were focused on the dynamics of sub-rotor and rotor circulations. The measurement program for SRP took place in 2004 and for T-REX in 2006. During T-REX, COAMPS was run in real time at high resolution (2 km grid increment) and the forecasts were used to select observing periods and for mission planning for three research aircraft taking measurements above the Sierra Nevada Range. In other studies, air-sea interaction in the Adriatic Seas was explored using the COAMPS/NCOM one-way and two-way coupled system. The coupled simulations demonstrate that the atmospheric winds and temperature were more accurately forecasted in a two-way coupled mode than with one-way coupling. The dynamics of several cases involving orographically forced flows during the Mesoscale Alpine Programme (MAP) were studied. The results of these simulations have led to a more complete understanding of gravity waves in three dimensions and their interactions with the boundary layer. High-resolution forecasts using COAMPS were used as part of the ONR Coupled Boundary Layers/Air-Sea Transfer (CBLAST) field experiment that led to improvements in the performance of near-surface temperature and winds forecasts.

Significance: COAMPS will play a significant role in providing atmospheric forecasts in support of Navy missions involving the deployment of weapons systems, strike warfare, radar propagation, and search and rescue. Research and development performed at HPC sites have led to measurable improvements in the predictive skill of COAMPS that will benefit the operational performance of COAMPS. The HPC sites will be the primary computing resources in FY2006 and beyond for the development of the fully coupled COAMPS system.

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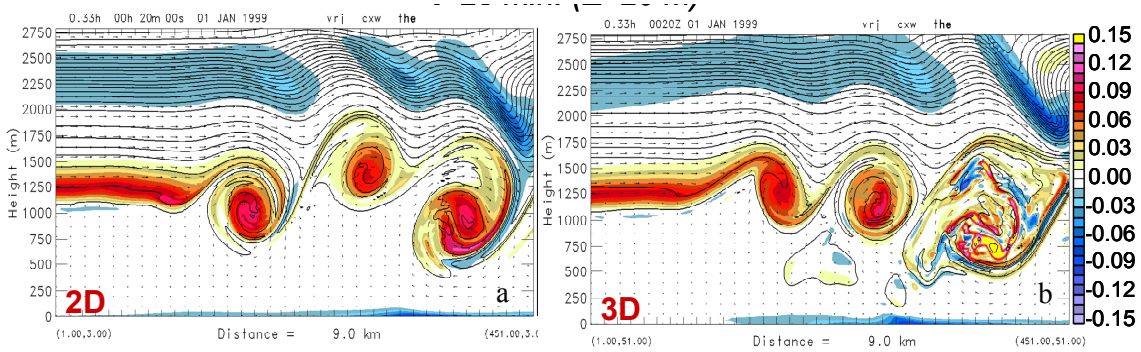


Figure 1. Vertical cross section of wind vectors, potential temperature (K) and y-component of the horizontal vorticity (s^{-1}) (color scale shown at right) for (a) two-dimensional simulation of sub-rotors and (b) three-dimensional simulation after 20 min. The horizontal and vertical grid increments are 20 m. Tick marks along the abscissa are shown every 250 m.

Title: Eddy-resolving Global and Basin-Scale Ocean Modeling
Author(s): Alan J. Wallcraft, Harley E. Hurlburt, and Jay F. Shriver
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P655 [NAVO, MS]; HP Opteron Cluster [ASC, OH]; Cray XT3, Compaq SC45 [ERDC, MS]

Research Objectives: Modeling component of a coordinated 6.1-6.4 effort on the "Grand Challenge" problem of eddy-resolving global and basin-scale ocean modeling and prediction. This includes increased understanding of ocean dynamics, model development, model validation, naval applications, oceanic data assimilation, ocean predictability studies, observing system simulation studies, and nested models.

Methodology: The appropriate choice of vertical coordinate is a key factor in OGCM design. Historically, we have used the NRL Layered Ocean Model (NLOM) because of its efficiency in computer time per model year. Layers are optimal for deep water but not for coastal domains, so as more computer power becomes available we are transitioning to models with hybrid vertical coordinates. The NRL Coastal Ocean Model (NCOM) allows both terrain-following and Z-levels in the vertical, and HYCOM has a completely general vertical coordinate (isopycnal, terrain-following, and Z-level) via the layered continuity equation.

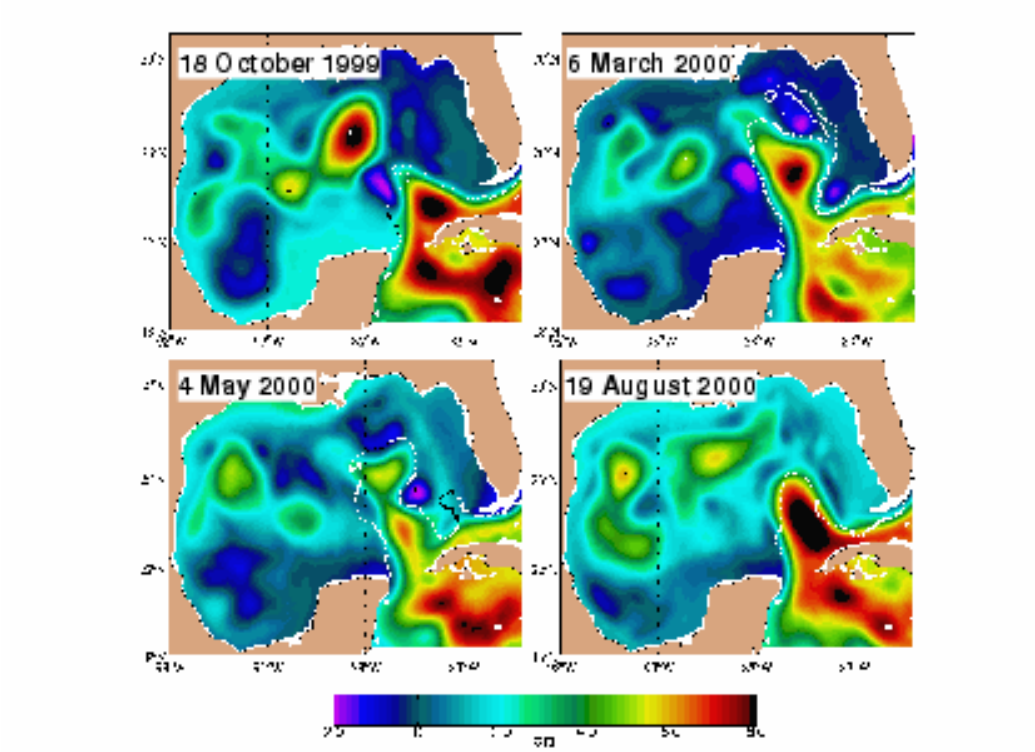
Results: 26 publications (submitted to in print) excluding abstracts, 22 refereed.
Global modeling: The fully global NCOM system with 1/8 mid-latitude resolution has been run daily by NRL in near real-time since November 2001, and was made operational at NAVO on 19 Feb 2006. It assimilates 3-D T\&S fields derived via MODAS synthetics from NLOM 1/16 or 1/32 SSH and MODAS2D 1/8 SST. See: http://www.ocean.nrlssc.navy.mil/global_ncom for real-time and archived results. Evaluation of results from several global NCOM experiments has continued. The 1/32 near-global upgrade to the existing NLOM 1/16 system has been running in near real-time since Nov 2003, and was made operational at NAVO on 6 Mar 2006 as a replacement for the 1/16 degree NLOM system. Real-time and archived results can be seen at: http://www.ocean.nrlssc.navy.mil/global_nlom}. 1/16 global NLOM was also run as a linear model to test the response to wind speed corrections using the QuikScat scatterometer. Development of 1/12 global HYCOM began last year and continues this year under DoD Challenge. Outside DoD Challenge, we ran at 0.72 globally to test different mixed layer models, reference ocean states, number of layers, layer structure, and corrections to the atmospheric forcing. We also used 0.72 and 1/12 Arctic-only regions to test sea-ice issues. This includes the CICE sea-ice model coupled to HYCOM, initially one-way coupling with planned extension to 2-way coupling and to a fully global coupled HYCOM-CICE system.

Data Assimilation: An upgrade to NCODA data assimilation is under development and evaluation in the Gulf of Mexico, and initial testing is underway in 1/12 global HYCOM under DoD Challenge.

CONESTS: Configured a 1/25 Gulf of Mexico HYCOM domain nested inside the 1/12 HYCOM Atlantic. It is now running with and without NCODA data assimilation. This domain is also being used by the SEED project to investigate the dynamics of the cross-shelf exchange, including the response of 1/25 Gulf of Mexico HYCOM to Hurricane Ivan in comparison to SEED observations.

Significance: Data Assimilative eddy resolving models are important components of global ocean monitoring and prediction systems. Military and civilian applications include ship routing, search and rescue, antisubmarine warfare, coastal and mine warfare, fisheries forecasts, pollutant spill risks, El Nino forecasting, ocean observing system simulation, and global change studies.

HYCOM/NCODA assimilation of real SSH, SST & XBT profiles



HYCOM nowcast SSH with the NAVO frontal analysis of MCSST observations (white/black lines, black data > 4 days old).

Title: Data Assimilation Studies
Author(s): William Campbell, Nancy Baker, Clay Blankenship, Benjamin Ruston, and Liang Xu
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: Linux Networx Cluster [ARL, MD]; SGI Origin 3900 [ASC, OH]; IBM P4 [NAVO, MS], [ARSC, AK]

Research Objectives: The research objective of this project is to investigate methods to improve our use of remotely sensed data for global and mesoscale numerical weather prediction, and to test and refine the NRL four-dimensional variational (4DVar) data assimilation system. Specific tasks include (a) improved modeling of surface emissivity over land to allow use of lower peaking channels in more areas of interest to the Navy and DoD, (b) experiments with correlated observation error and higher observation densities to develop intelligent data thinning strategies for the extremely high volume of remotely-sensed data available in the coming NPP and NPOESS eras, and (c) development and testing of new bias correction methods that can accomodate model error.

Methodology: Several researchers will conduct experiments for the data assimilation project, using a common fixed dataset consisting of a complete suite of observations, including AMSU-A, AMSU-B, HIRS3, SSMIS, and AVHRR radiance data, for two winter months and two summer months. Cycling data assimilation runs with long forecasts affords a semi-operational environment in which to test many possible improvements to NRL Atmospheric Variational Data Assimilation System (NAVDAS) and its four-dimensional generalization, NAVDAS-AR (Accelerated Representer).

Results: A large dataset of all meteorological observations needed for two months of cycling data assimilation have been ported and archived on all the HPC machines. We are in the process of porting the NAVDAS code and rewriting run scripts so that they can run appropriately in the HPC queuing environments. Tests on our local SGI Origin 3000 machines, using the TAU profiling system, confirm that NAVDAS scales nearly linearly up to 60 processors, and we are confident tht it will continue to scale well with even more processors. As soon as our code compiles and runs on individual HPC machines, our scientists will begin their cycling data assimilation experiments.

Significance: The importance of METOC to the Navy and DoD is well known. For example, a significant increase in forecast skill was shown in both the transition of NAVDAS to operations at FNMOC, and the transition of direct radiance assimilation of AMSU-A data. The density of conventional observations is not likely to increase apreciably; the future of data assimilation is remotely-sensed data. Our research further improves NAVDAS, helps prepare for the extremely large satellite data volulmes of the NPOESS era, and lays the foundation for the future in NAVDAS-AR.

Title: Development of a Middle Atmosphere in the Navy Operational Global Atmospheric Prediction System (NOGAPS)
Author(s): Lawrence Coy[1], Stephen D. Eckermann[1], John McCormack[1], David Siskind[1], Gerald Nedoluha[1], Karl Hoppel[1], Andrew Kochenash[1], Jun Ma[1], and Douglas R. Allen[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]Dordt College, Sioux Center, IA
CTA: CWO

Computer Resources: SGI Origin, [ASC, OH], [ERDC, MS], [SMDC, AL]; SGI Altix [NRL, DC]; IBM P4 [NAVO, MS]

Research Objectives: For FY06, the aim of the project is to test and develop an extended altitude version of the Navy's operational weather forecast model, NOGAPS-ALPHA (Navy Operational Global Atmospheric Prediction System- Advanced Level Physics High Altitude) in support of 6.1 ARI (Atmospheric Coupling; David Siskind, PI) and 6.2 new start (Data Assimilation: Gerald Nedoluha, PI) research. The inclusion of altitudes up to 100 km requires new physics for radiative heating, tracer transport (including ozone), and sub-model resolution parameterizations. Understanding the complex interactions among physics parameterizations along with the effects of the increased vertical domain requires the integration of the complete forecast system, often at high spatial resolution, for times up to several months or more. The experiments are designed around careful changes to the code and results are compared with control runs and independent calculations in judging the success of the changes and their potential for integration into the operational NOGAPS code.

Methodology: The NOGAPS-ALPHA atmospheric circulation model solves for the future state of atmosphere through time integration of the hydrostatic meteorological primitive equations on a sphere. The Fortran 90 NOGAPS code makes heavy use of MPI for parallel processing. Typically 20-80 processors are used for development runs: however, the code scales well and over 200 processors are used when the model is run operationally. Model time steps are in the range of 1 to 5 minutes. The atmospheric state at a given time requires on the order of one million numbers for its specification. Large amounts of output storage are needed for some experiments. We also interface to NOGAPS-ALPHA and run NASA Global Modeling and Assimilation Office's ozone data assimilation system (DAS) code and the NAVDAS (Navy Atmospheric Variational Data Assimilation System) code.

Results: In FY06, we have developed, tested, and compared ozone photochemistry parameterization schemes, including one scheme we created based on NRL's two-dimensional chemistry model, CHEM2D-OPP (Ozone Photochemistry Parameterization. We have added high altitude radiative cooling code to NOGAPS-ALPHA. We have also developed the ability to assimilate ozone observations using NAVDAS. Ozone data assimilation based on the GOATS (Global Ozone Assimilation Testing System) has continued and is near publication. NOGAPS-ALPHA hindcasts of resolved gravity waves have been compared to corresponding satellite observations, and NOGAPS-ALPHA forecasts have been used to study the response of the global atmosphere to a total solar eclipse.

Significance: This research directly supports on NRL's 6.1 ARI atmospheric coupling program by extending NOGAPS through the middle atmosphere (altitudes~15-100 km), and NRL's 6.2 data assimilation new start by using NOGAPS-ALPHA with NAVDAS and GOATS to assimilate higher altitude ozone and temperature satellite data. Changes resulting from this research will be progressively transitioned into the operational NOGAPS to address the Navy's need for improved weather forecasts at all altitudes and real-time specification of the atmosphere from ground to space. For example, CHEM2D-OPP, the ozone photochemistry parameterization scheme developed at NRL-DC as part of this HPC project has been incorporated into NOAA's operational forecast system, the main weather forecast system for the US and has been transitioned to FNMOC's operational forecast system.

Title: Global Ice Modeling
Author(s): Pam Posey, Alan Wallcraft, Joe Metzger, and Lucy Smedstad
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM P4 [NAVO, MS]; SGI Origin [ERDC, MS]

Research Objectives: (1) to contribute to the development of the next generation Navy coupled ice-ocean model, (2) to test the new Navy Polar Ice Prediction System 3.0 (PIPS 3.0) model on computers compatible with the types of machines that will be available at the Navy operational centers, and (3) to gain an understanding of seasonal and inter-annual variations of coupled ice-ocean systems in the Arctic and its marginal seas.

Methodology: The overall approach is to take advantage of recent model improvements to eddy-resolving, hybrid-coordinate global ocean models (such as NCOM and HYCOM) and to ice models (the viscous-plastic Hibler and elastic-viscous-plastic LANL model). These improvements embraced numerical schemes, model physics, small-scale parameterization, ridging scheme and adaptation to massively-parallel machines. A major effort during this year was coupling CICE (PIPS 3.0) to global NCOM and HYCOM. Model physics verification will include testing the effect of particular choice of ice rheology and thermodynamics, and the nature of atmospheric forcing (wind stress over ice, prescribed vs. bulk heat flux formulas, feedback effects, etc.) Simulations and process studies include runs on both seasonal and inter-annual time scales. The effect of atmospheric forcing on the ice-ocean model codes is examined by running multi-year simulations (2-5 years) to evaluate the development of ice thickness and ice concentration. The main verification data sets for ice come from SSMI microwave data on ice concentration, Arctic buoy data on ice motion, and submarine sonar data on ice-thickness.

Results: The LANL CICE model was chosen for the new PIPS 3.0 based on its advanced ice thickness structure (multi-level), EVP ice rheology, ice ridging and its improved thermodynamics. The purpose of the new PIPS 3.0 is to forecast a better representation of the ice edge, ice drift and to provide guidance for determining areas of lead formation. A high resolution (9 km) and multi-level ice thickness formulation should provide the means to predict areas of possible lead opening and closing and improved ice edge growth/decay. During this year, the LANL CICE model was tested on an Arctic grid, similar to that used in the PIPS 2.0 model but at higher resolution (9 km vs 25 km), that was coupled to a climatic ocean. Several simulations were run with the recent five full years of NOGAPS forcing, 1999-2003 to finalize the code to be used for coupling to the Navy ocean models. Test cases focused on modifying the initial ice conditions to generate a realistic sea ice cover to initialize the coupled model runs. During FY06, the NCOM salinity, temperature and ocean current fields were used in the PIPS 3.0 code replacing the climatic ocean fields. This was tested using NCOM fields for the year 2003. Also during this year, the LANL CICE (version 4.0 – ESMF code) was run on a HYCOM coarse grid (35 km) using five years of NOGAPS forcing, 1999-2003. Figure 1 represents the 2003 March monthly mean ice concentration using the CICE (ice-only) model, the NCOM/CICE and the SSMI observations.

Significance: This project is applied to the testing and validation of existing sea ice forecast systems and the development of new systems. In addition, this project provides insight into the ice and ocean circulation of the Arctic both regionally and in the global sense.

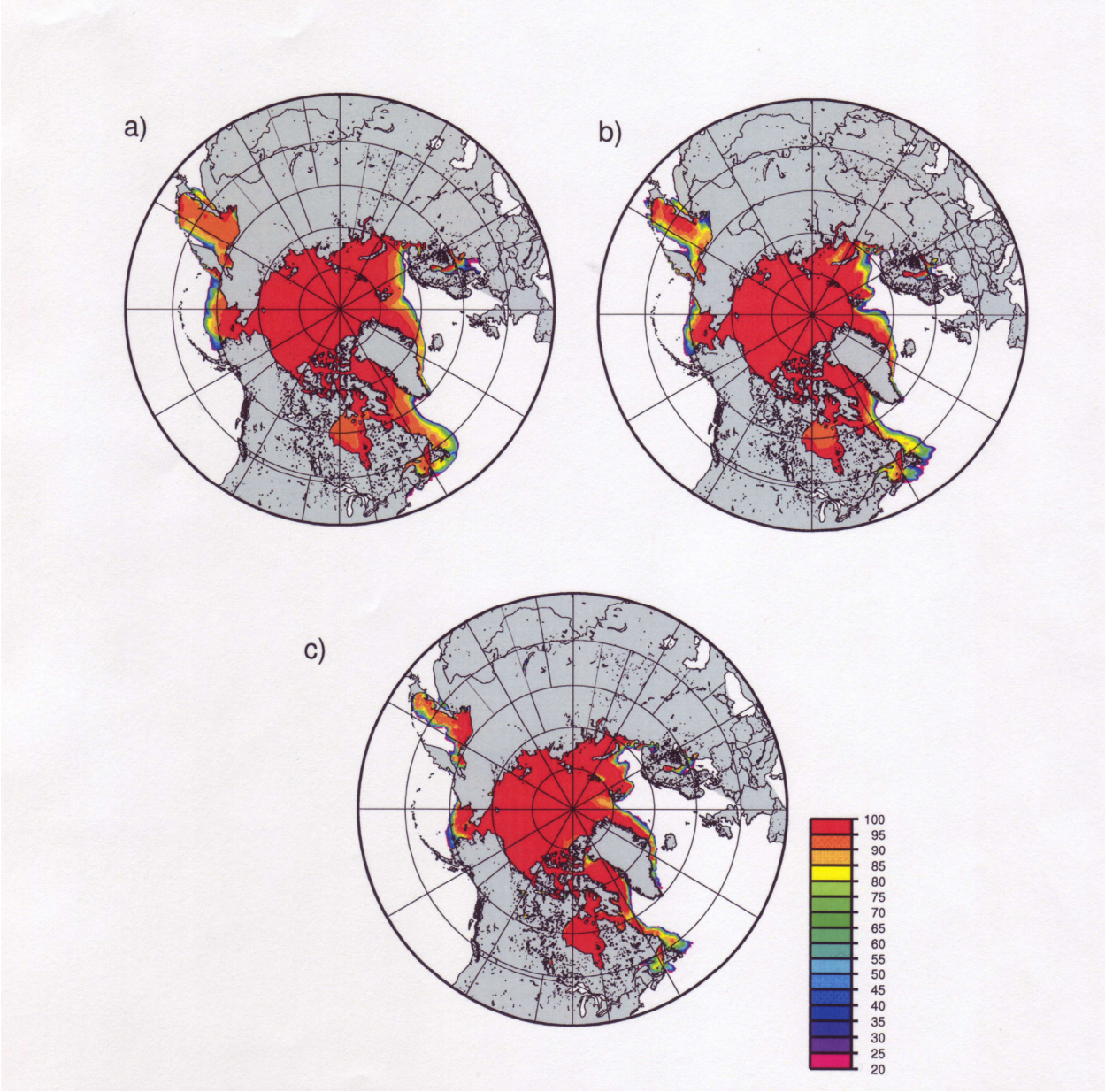


Figure 1. March 2003 mean ice concentration (%) for (a) CICE (ice-only) grid, (b) NCOM/CICE grid and (c) SSM/I observations. The coupled NCOM/CICE (b) shows a more realistic ice edge as compared to the SSM/I (c).

Title: Finite Element Coastal Modeling
Author(s): Cheryl Ann Blain
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

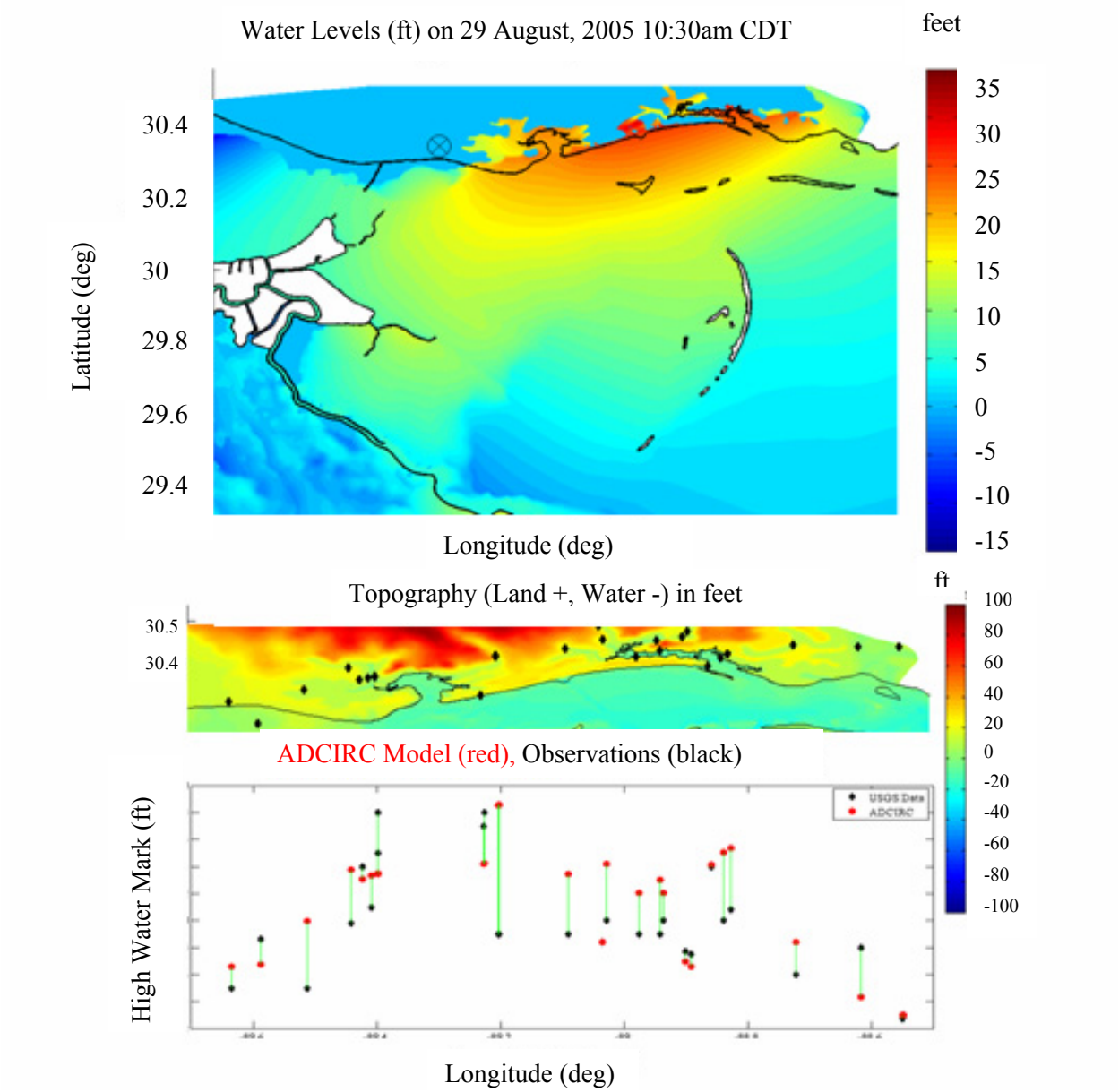
Computer Resources: IBM P4 [ARL, MD], [NAVO, MS]

Research Objectives: The objectives are to more fully understand and predict the complex dynamical processes occurring in coastal waters through the development and application of advanced, finite element-based numerical coastal ocean models. The bulk of the high performance computing work undertaken this FY has focused on realistically capturing storm surge and inland inundation processes.

Methodology: The finite element coastal circulation model, ADCIRC, has a successful history of accurately modeling the development and propagation of storm surge generated by hurricane force winds [e.g., Blain et al., 1994; 1998; Westerink et al., 2005]. The two-dimensional option of the ADCIRC model is capable of representing the barotropic dynamics generated by tides, winds, waves and river inflow. The computational mesh over which the model is run is composed of linear triangular elements that offer unequaled flexibility with respect to the representation of geometric complexities and is particularly well suited to capturing coastal processes that respond to highly variable bathymetry or topography. For storm surge applications, inland inundation is an important process. As was seen during the recent disaster caused by Hurricane Katrina in August of 2005, the accurate prediction of coastal inundation can mean the difference between life and death. The detailed representation of water movement over bathymetric features that include barrier islands, coastal protection structures, inland waterways, and river channels presents new computational challenges as the constructed meshes aim to resolve the multiple spatial scales present in large coastal-shelf systems such as was applied to Katrina's storm surge.

Results: The generation and propagation of storm surge resulting from Hurricane Katrina was simulated by the ADCIRC model. The Mississippi Gulf Coast and southeast Louisiana including Lake Ponchartrain and the MS River have been represented by a mesh of 703,431 unstructured triangles (375,479 nodes) that extends from the Mississippi coastal region out into the Gulf of Mexico and beyond into north Atlantic ocean waters. The large computational domain permits the realistic generation of hurricane storm surge inside the domain and allows for proper treatment of the resonant modes in the Gulf of Mexico. The near coastal waters and inland topography of the Gulf coast is captured at a spatial resolution on the order of 225 m. Simulations are forced by tides at the boundary in the deep Atlantic ocean as well as internally. Surface wind stress forcing is obtained from the NOAA Hurricane Research Division Katrina reanalysis product (http://www.aoml.noaa.gov/hrd/Storm_pages/katrina2005/wind.html) for the period 28 Aug.18 Z to 29 Aug. 17 Z 2005. A 17.7-day simulation (including a 15-day tidal ramp-up period) having a time step of 1 second required 12 CPU hours using 128 processors on the NAVO IBM-P4. Comparisons between computed high water marks and USGS recorded values indicate an absolute mean error of 3 ft. This discrepancy is rather small considering that wave contributions to the surge were neglected. Following directly from this work was the development of an operational hurricane storm surge forecasting capability based on the ADCIRC model transitioned to NAVOCEANO at Stennis Space Center, MS, and a more detailed examination of the performance of the inundation algorthm used within the ADCIRC model over a series of idealized beaches.

Significance: Detailed knowledge of currents and water levels in inundated areas are needed for both operational planning and successful execution of Navy SEAL and Special Boat Unit riverine missions. Non-naval interest in high resolution currents and water levels in riverine and coastal environments relates to sediment transport, search and rescue operations, pollutant dispersal, and coastal restoration.



Storm surge and inundation along the Mississippi gulf coast predicted by the ADCIRC model 30 minutes after the landfall of Hurricane Katrina on August 29, 2005. Comparisons to 27 USGS high water marks reveal an average model error of 3 feet, an excellent result considering the coarse 225 m inland resolution and the neglect of wave effects.

Title: Coupled Ocean-Acoustic Dynamics
Author(s): A. Warn-Varnas, S. Piacsek, and T. Campbell
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

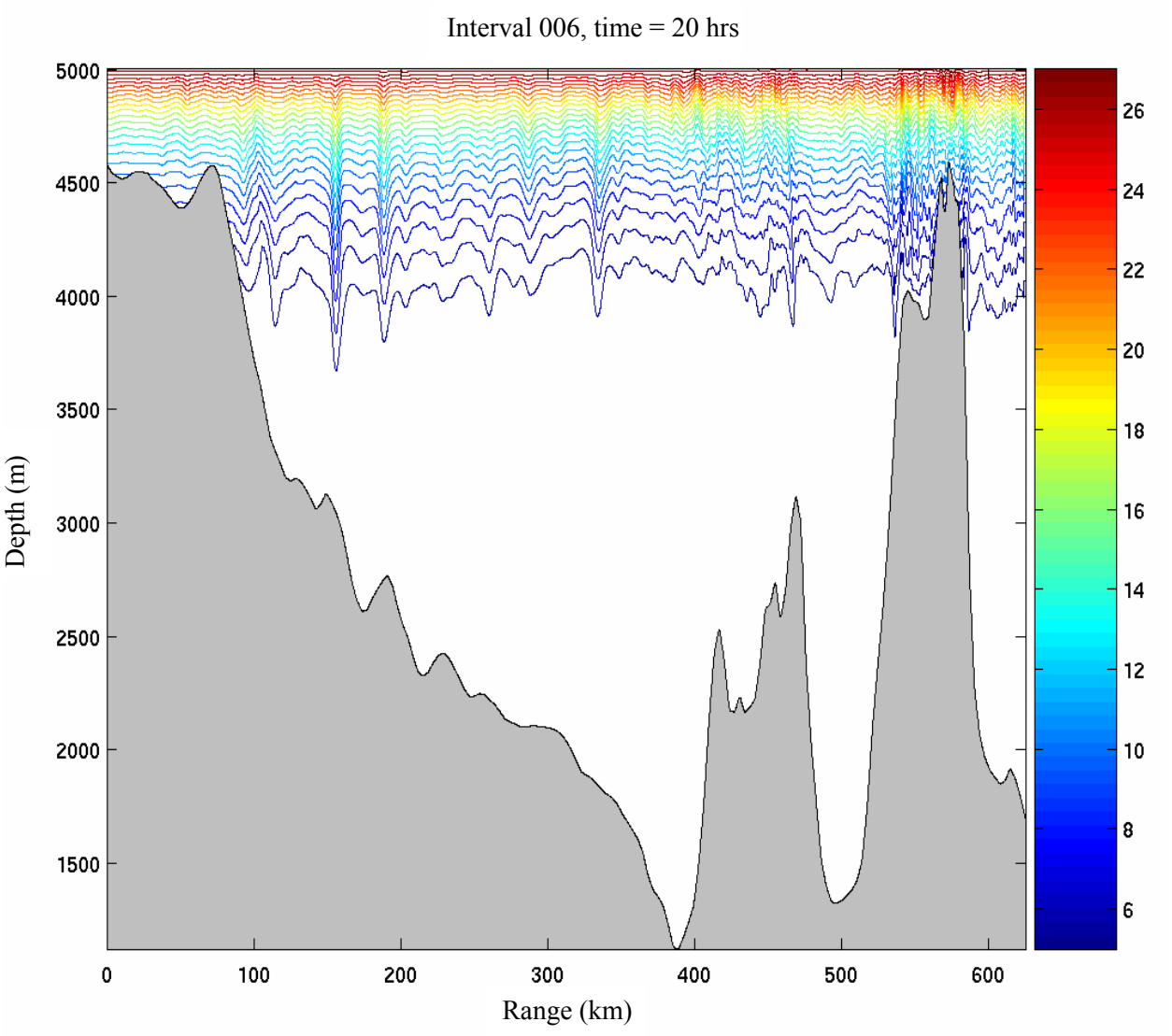
Computer Resources: IBM p655 and P4 [NAVO, MS]

Research Objectives: The principal goals of this project are to acquire an in-depth understanding of how changes in ocean parameters couple into changes in acoustic propagation, and to exploit this understanding to develop much more efficient 4-D ocean acoustic predictions. Specific goals include (a) the understanding of the generation and propagation of solitons in the Yellow Sea, and the Straits of Messina and Luzon; (b) an understanding of how changes in ocean parameters couple into changes in acoustic parameters; (c) the exploitation of this understanding for generating more efficient 4-D ocean acoustic predictions, and (d) to search with coupled ocean-acoustic models for losses and enhancements of acoustical energy and to explain the loss and enhancement mechanisms.

Methodology: Perform joint ocean-acoustic modeling with very high resolution soliton models, with grid spacings of a few meters in the vertical and tens of meters in the horizontal. Among the models employed will be the 2.5 D nonhydrostatic sigma coordinate model of Lamb (1994) and the 3D nonhydrostatic sigma-coordinate model of Smolarkiewicz (2001). These models predict the soliton signal in terms of temperature, salinity, and current. The local soliton models will be nested in temperature and salinity fields derived from data or the MODAS-NCOM data-assimilative model results. Tidal forcing will be provided from barotropic tidal models or tidal data bases. The calculated sound speeds from oceanographic predictions will be used in acoustical field calculations for various environmental situations.

Results: The relation of soliton packet wavelengths to acoustical modes, and the loss of acoustical signal due to soliton packets, has been investigated. The shoaling of soliton packets, effects of geographic boundaries and curvature signature of the soliton packets (surface divergence and convergence) have also been studied. An examination of predictability statistics and three-dimensionality of the problem has also been initiated. The results of FY06 convergence studies on horizontal resolution have shown that for excellent results we need resolutions of $100m < dx < 250m$, but adequate representations of the physics occur with $dx \sim 500m$ and marginal ones with $dx=1000m$. A threshold tidal magnitude for the generation of solitary wave trains has been found, and the examination of the effects of the initial density profiles and tidal amplitudes has been continued. Studies using the EULAG model have also been extended to the lock exchange problem and the DJL analytic soliton solution as part of benchmarking against other nonhydrostatic codes, and to the effects of the full 3D topography in the Yellow Sea.

Significance: MCM, Special Warfare, UAV's and shallow water acoustics are affected by interaction with solitary wave trains.



Predicted temperature in mid-plane South China Sea & Strait of Luzon region with 3D nonhydrostatic Smolarkiewicz EULAG model. Large amplitude internal bore (~ 240 m) propagating towards the Chinese continental shelf.

Signal Image Processing

- Extraction of useful information from sensor outputs (sonar, radar, imaging, signal intelligence (SIGINT), navigation) in real time.

- Usually such processors are abroad deployable military systems and hence require ruggedized packaging and minimum size, weight, and power.

- Research, evaluation, and test of the latest signal processing concepts directed toward these embedded applications.

Title: Automatic Classification of Hyperspectral and Multi-Sensor Remote Sensing Imagery
Author(s): Charles M. Bachmann and Robert A. Fusina
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: SIP

Computer Resources: Linux Networx Cluster [ARL, MD]; Atipa Linux Cluster [SMDC, AL]

Research Objectives: The project emphasizes the development and evaluation of novel algorithms for automatic detection and classification, with particular emphasis on hyperspectral, multi-spectral, radar (synthetic aperture radar), and multi-sensor and multi-temporal imagery.

Methodology: We continue to focus this year on the development of scalable data-driven models of nonlinear structure in high-dimensional remote sensing data, such as hyperspectral imagery. To date, data-driven analysis of hyperspectral imagery has been dominated by linear methods. Although linear methods are powerful tools, they do not model effectively known sources of nonlinearity in hyperspectral imagery. On land, these nonlinearities arise in vegetative canopies because of multi-path scatter and bi-directional reflectance distributions (BRDF effects). In aqueous environments, for example littoral waters or marshes, other nonlinearities appear because water is a highly nonlinear, attenuating medium with both direct and diffuse scattering mechanisms within the water column. The data driven methods that we explore in this effort optimize a set of intrinsic manifold coordinates that parameterize nonlinear structure directly.

Results: Using HPC resources, we were able to demonstrate an improved methodology for achieving scalable manifold coordinate representations. The new method removes artifacts present in our original methodology. With the new approach, we were able to demonstrate the optimization of a seamless manifold coordinate product on coastal hyperspectral scenes of size $O(10^6)$ pixels or greater. Several applications areas such as bathymetry retrieval, land-cover classification, and anomaly detection were also explored. For example, specifc tests of bathymetric retrieval with manifold coordinate representations were conducted using airborne hyperspectral imagery of the Indian River Lagoon, FL, taken by the NRL PHILLS hyperspectral sensor in July 2004. Manifold coordinate representations of the data were used to generate compact look-up tables that were associated with known depths from SHOALS LIDAR measurements conducted within a few months of the PHILLS flights. Results showed that a scene-independent product could be derived with acceptable error tolerances.

Significance: Nonlinearities in hyperspectral imagery impose fundamental limitations on performance for the linear methods frequently used to analyze hyperspectral imagery. Manifold coordinates, which provide a direct data-driven representation of inherent nonlinearities in hyperspectral imagery, have the potential to revolutionize how hyperspectral imagery is processed, and improve the accuracy and fidelity in important application areas such as anomaly detection, automatic target recognition, change detection, precision mapping of land-cover, and the development of in-water products.

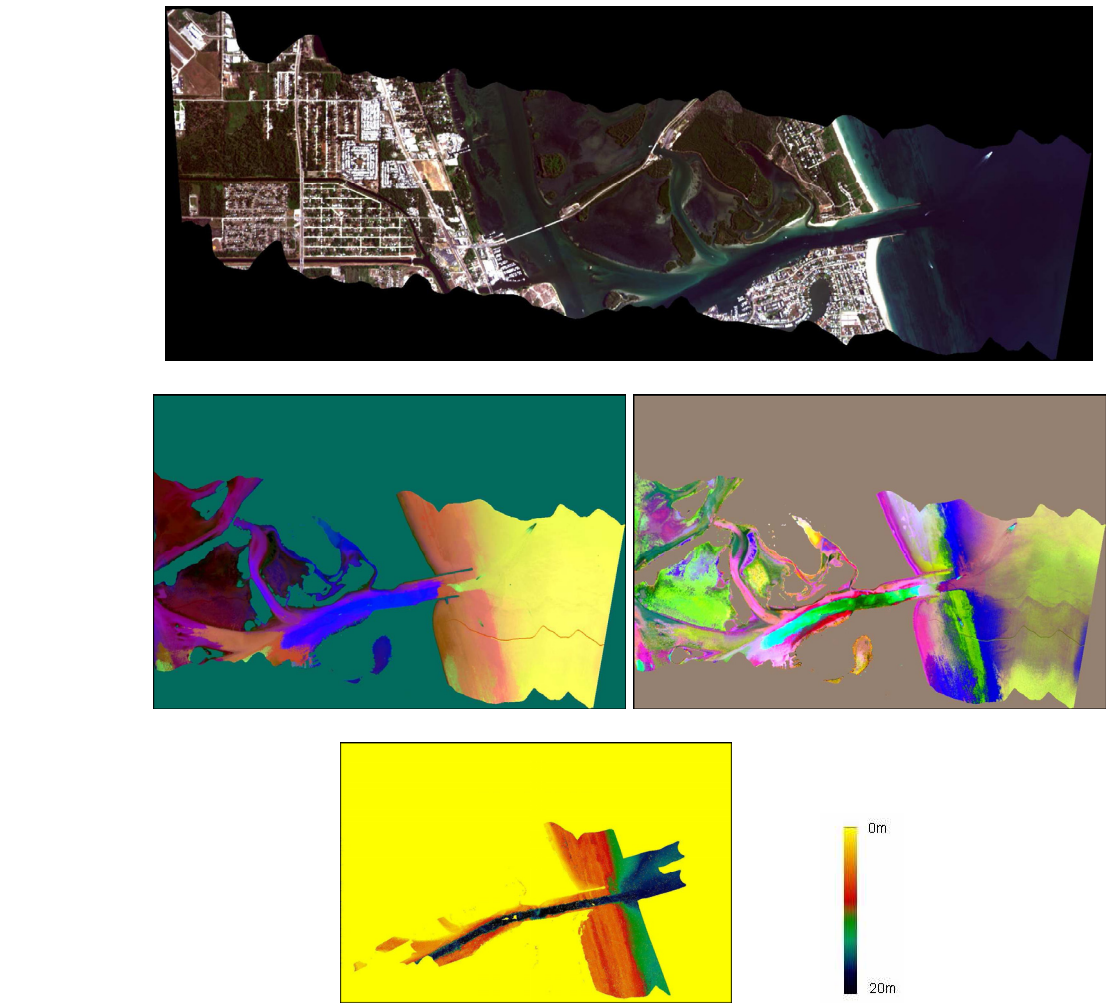


Figure 1. (Top) NRL PHILLS hyperspectral image (HSI) from Indian River Lagoon, Florida, July 14, 2004. (Second row) Some of the manifold coordinates (water pixels only, in vicinity of LIDAR survey) derived from the HSI and represented here as RGB: (left) components 1-2-3, (right) components 14-15-16. (Third row) Retrieved bathymetry based on HSI manifold coordinate LUT (table with 75,000 entries) associating manifold coordinates with SHOALS LIDAR measurements taken four months apart from PHILLS flights. (Bottom) Results for test pixels, comparing HSI manifold coordinate retrieved depth and LIDAR derived depth: (left) within scene (test pixels not in LUT), (right) for a test scene roughly 60 km away on a different day (July 15, 2004).

Environmental Quality Modeling and Simulation

- High-resolution, three-dimensional Navier-Stokes modeling of hydrodynamics and contaminant and multi-constituent fate/transport through the aquatic and terrestrial ecosystem and wetland subsystems, their coupled hydrogeologic pathways, and their interconnections with numerous biological species.

- Used for stewardship and conservation of natural and cultural resources, optimal design and operation of installation restoration, and enhancement alternatives and development of short- and long-term strategies for integrated management in support of installation environment quality.

- Work in the area of noise evaluation and abatement as well as water quality models.

Title: Remote Sensing of Surface and Sub-surface Oceanic and Terrestrial Features
Author(s): S. R. Chubb[1], A. L. Cooper[1], J. A. Toporkov[1], R-Q. Lin[2], and Charles Tilburg[3]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]NSWC Carderock (DTRC), MD; [3]University of Georgia, Athens, GA
CTA: EQM

Computer Resources: SGI Origin 3000 [ERDC, MS]; SGI Altix [NRL, DC]

Research Objectives: To develop, improve and apply algorithms for monitoring and detecting the behavior of features on and below the surface of the ocean or land, by comparing remotely sensed images and measurements with simulations, using optical and microwave, active sensors, and passive gravitational and magnetic sensors. Particular oceanic features of interest include the behavior of waves and surfactant evolution in the presence of wind on the ocean surface, near surface and sub-surface currents, and the effect that changes in bottom topography have on surface and near-surface waves. Terrestrial features of interest include variations in surface and near-surface topography, inferred from air-borne platforms.

Methodology: Variations in surface and near-surface terrestrial topography (including changes in materials below the surface) are inferred from simulations of the local gradient of the gravitational force, using advanced forms of gravity gradiometers, involving Cold and Ultra Cold neutral Rubidium atoms. Here, simulations are initialized by confining Cold Atoms and Ultra Cold Atoms (Bose Einstein Condensates) to a particular potential well of a periodic lattice (referred to as an Optical Lattice), that is formed from the interaction of the atoms with standing waves of light that result from coherent, counter-propagating, Laser Fields; while gravitational gradients are inferred from the subsequent time history of the tunneling between neighboring wells when the atoms are subjected to an outside gravitational force. The simulations are initialized from the eigenstates and band structure, from a 1-Dimensional Optical Lattice, in the absence of gravity. In the case of wide Laser Beams, because the atoms remain confined, these states can be computed from strictly 1-Dimensional solutions of the Schroedinger Equation (which, for, low densities, is Mathieu's equation). While in more realistic cases involving thinner Laser Beams, the atoms are held within the Optical Lattice in directions perpendicular to the beams, using harmonic wells from external, D.C. magnetic fields. Here, solutions are derived variationally from a mixed basis set, involving products of Wannier states (constructed from the 1-dimensional Mathieu's equation), with (Hermite polynomial) solutions of the 2-dimensional (axially symmetric) Harmonic oscillator potential. The subsequent time evolution is computed using the Cayley method (a variant of the Crank-Nicholson procedure). In modeling oceanic features, we include the effects of the wind, currents, and bottom topography on radar imagery and Doppler Spectra (DS) by simulating the impact these effects have on the ocean surface and in the resulting electromagnetic backscatter. Here, various types of surface wave fields and models are used. Winds and currents in the open ocean are modeled from the growth and dissipation of a broad spectrum (BS) of surface waves. The backscatter from these wave-fields is derived from the spectral density S, through the wave-action equation, using a 4-dimensional numerical grid (involving two spatial and two spectral degrees of freedom). We do this using either the Erim Ocean Model (EOM), or the NRL Time-dependent Ocean Wave model, from currents derived from either the Princeton Ocean Model, ECON3d model, or inferred from observation or in situ measurements.

Results: Some simulations were conducted of ocean features and radar imagery. A theoretical breakthrough involving the identification of an optimal form of gravimeter (resulting from differential edge effects associated with losses of atoms in a Bose Einstein Condensate), led to a new form of simulation, involving systematically altering an applied acceleration of the optical lattice in a way that will allow precise measurements of gravity.

Significance: Research has application in ASW/UT, MCM, Space Surveillance, environmental monitoring and is important in the tactical problems of extracting bathymetry and using remote sensors.

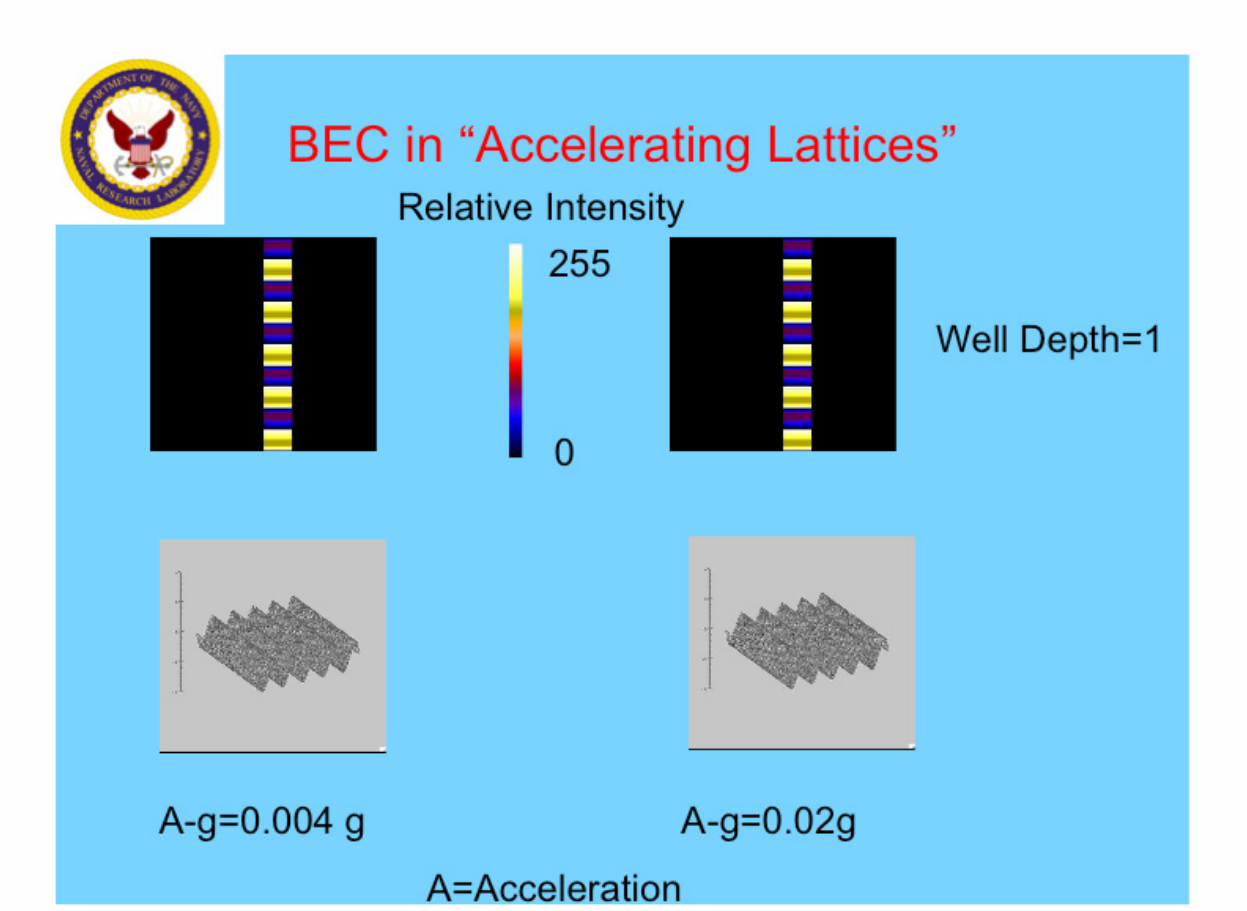


Figure 1. Three-Dimensional simulations of a common relative adsorption image intensity from an Atomic Bose Einstein Condensate, initialized at a common time. (The Bose Einstein Condensate (BEC) adsorption image intensity is required to oscillate in time). As a function of time, each image in the simulation to the left is almost identical to the simulation on the right, but the oscillation has a considerably longer period (a factor of five greater). However, the images are actually not quite identical. Near the end of each complete period, a small variation in intensity occurs that is most pronounced along a vertical line in the middle of each BEC (i.e., in the middle of each colored portion of the two images at the top of the figure). This variation in intensity, which is the result of small loss of atoms from the BEC, resulting from edge effects can be precisely predicted as the acceleration (A) of the approached gravitational constant (≈ 9.8 m/s^2).

ENS

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- Uses include passive and active devices, detectors, emitters, and their physical integration and architecture.

- ENS provides support for emerging electronic technologies, design tools, and computing paradigms such as reconfigurable computing and specialized hardware.

Title: Numerical Studies of Semiconductor Nanostructures
Author(s): T. L. Reinecke, S. Badescu, L. M. Woods, and R. Rendell
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: ENS

Computer Resources: SGI Origin 3000 [ASC, OH]; SGI Altix [ASC, OH]; HP-XC [ASC, OH]

Research Objectives: To calculate the geometrical structures and the electronic properties of adsorbates on carbon nanotubes for applications as chemical sensors. To understand the electronic and optical properties of realistic semiconductor nanostructures for use in quantum information technology.

Methodology: *ab initio* electronic calculations are used for the electronic and structural properties of adsorbates on nanotubes. Numerical boundary element method calculations for single particle properties, and many-body techniques for the effects of interactions between excitations are used for semiconductor nanostructures in quantum information technology.

Results: Highlights of this year's work include:

Ab initio calculations are being used to study the adsorbate atoms on carbon nanotubes. LDA at the GGA level is being used for the electron-electron interactions, and structures are obtained by total energy minimization. Calculations have been made for benzene adsorbed on nanotubes and for benzene functionalized with NH_2, CH_3 and NO_2 on nanotubes. We find that these closed shell systems physisorb on nanotubes and do not change the nanotube electronics properties significantly. This work is in press in Physical Review B.

Ab initio calculations have been made for the adsorption of acetone and methanol on carbon nanotubes with and without carboxyl functionalization of the nanotube, which occurs on nanotube purification. We find that the adsorption is strong and the electronic properties of the nanotube are changed significantly only after carboxyl functionalization. This work has given rise to a new understanding of adsorption processes on nanotubes and to a new procedure for developing sensors based on nanotubes. This work has been published jointly with NRL experiment in Nanoletters.

A theory of spins in coupled quantum dots for implementations of two-qubit gates in quantum information has been developed, and detailed calculations have been made for realistic quantum dot systems. This work has been done in conjunction with NRL experiment. The theory includes carrier tunneling, Coulomb interactions and spin exchange, and detailed calculations have been made for vertically coupled InAs/GaAs quantum dot systems of interest to experiment. This work has been published jointly with experiment in Science and in Physical Review Letters.

Calculations have been made of the coupling between quantum dots and the photonic modes of micron sized semiconductor microcavities. In joint work with experiment, we have demonstrated for this first time strong coherent coupling between two quantum dots mediated by the cavity photon. Calculations have guided experiment and have been used to extract the true effects of dynamic cavity-quantum dot coupling from experiment. This work has been published in Nature and in Optics Letters.

Significance: An improved understanding of the interactions between adsorbates and nanotubes has provided the basis for a novel class of chemical sensors. Controlled coherent coupling between spins in quantum dots will form the basis for the two qu-bit gates from quantum dots needed for quantum computing. Strong coupling between quantum dots and microcavity modes can provide fast coupling between distant quantum dots and make possible architectures for distributed computing.

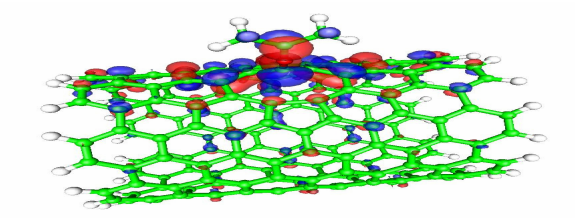

Figure 1. Highest occupied molecular orbital for acetone adsorbed at vacancy site on a carbon nanotube

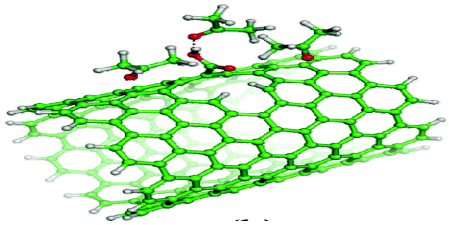

Figure 2. Structure of three acetones adsorbed at carboxyl defect on carbon nanotube

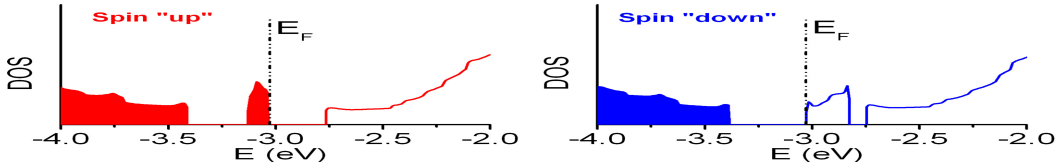

Figure 3. Electronic density of states for CH_3 adsorbed on a carbon nanotube from spin polarized density functional calculations

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Site Index

Major Shared Resource Centers (MSRC)

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